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- Biomolecular and Organic Electronics
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- Biotechnology
- Molecular Physics
- Regenerative Medicine
- Molecular Surface Physics and Nano Science
- Applied Sensor Science
- Surface Physics and Chemistry

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- Conservation Ecology Group
- Plant Evolution and Domestication Group
- The Sensory and Behavioral Physiology Group

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- Organic Chemistry
- Physical Chemistry
- Inorganic Chemistry
- Analytical Chemistry

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- Nanostructured Materials
- Plasma & Coatings Physics
- Semiconductor Materials
- Surface and Semiconductor Physics
- Thin Film Physics

## SCIENTIFIC BRANCH OF THEORY AND MODELING

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- Computational Physics
- Theoretical Biology
- Theoretical Physics

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- CeNano
- FunMat
- LiLi-NFM
- LBB
- SIMARC

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The Department of Physics, Chemistry and Biology (IFM) hereby presents its 42nd consecutive progress report since the start in 1970. The report contains a description of activities in research and education within the department and is intended as a source of information for colleagues and other interested readers.

IFM is organized in five scientific areas:
- Applied Physics
- Biology
- Chemistry
- Material Physics
- Theory and Modelling.

A large part of the research within these divisions is made possible by generous grants from founding agencies like The Swedish Research Council (VR), The Swedish Foundation for Strategic Research (SSF), VINNOVA, Formas, The Knut and Alice Wallenberg Foundation and internationally also through the European Research Council and the FP7 framework programme.

During the year 2012, a record high of 29 doctoral and 19 licentiate theses were presented. More than 230 undergraduate courses were presented in Master of Science in Engineering programmes, in Master of Science programmes, in Bachelor of Science in Engineering programmes, and in teacher training programmes.

The image on the cover shows a mirror-reflected experimental Valence Electron Energy Loss Spectrum line scan obtained across an Al$_{1-x}$In$_x$N multilayer structure grown on Al$_2$O$_3$. The spectrum intensity is represented by a color scale and each horizontal line corresponds to a local electron energy loss spectrum in the range 15 to 25 eV. The central layer corresponds to Al$_2$O$_3$, and it is surrounded by Al$_{1-x}$In$_x$N layers with step-wise increasing In-concentration.

More details of our research, graduate and undergraduate programmes can be found at www.ifm.liu.se.

Please also feel free to contact us by mail, e-mail or telephone.

Göran Hansson, Professor
Head of Department
Organization

ADMINISTRATION

Head of Department
Göran Hansson

Deputy Heads
Magdalena Svensson
Per Jensen
Inger Johansson
Louise Gustafsson Rydström
Bengt Andersson

DEPARTMENT BOARD

Members
Göran Hansson, Chairperson
Igor Abrikosov, Teacher representatives
Kenneth Järrendahl
Peter Nilsson
Johanna Rosén
Uno Wennnergren
Susanne Andersson, Techn/adm. representatives
Mattias Tengdelius, PhD stud. representatives
Martin Eriksson
Patrik Åkesson, Student representatives
Mats Werme
Patrik Hallsjö
Ingegärd Andersson, Secretary
Lena Martinsson

Personnel

Scientific areas

Applied Physics

Chemistry

Material Physics
- Functional Electronic Materials, Nanostructured Materials, Plasma and Coatings Physics, Semiconductor Materials, Thin Film Physics

Theory and Modeling
- Bioinformatics, Computational Physics, Theoretical Biology, Theoretical Physics

Divisions

Biology
- Ecology, Molecular genetics, Zoology

Chemistry
- Biology
- Chemistry

Material Physics
- Chemistry

Study Programmes

Ph.D. studies
- Biology
- Chemistry
- Physics – Engineering
- Physics – Natural Science
- Physics – Measurement Technology

Research Centra

AFM
- Biosensors and Bioelectronics Centre
- CeNano
- FunMat
- LiLi-NFM
- SIMARC

LSG, Local co-operation group

Central department functions

Personnel

Economy

Technical

Computer support

Research and Education
Undergraduate Teaching

AREA
Biology
Chemistry
Measurement Technology
Physics-engineering programs
Physics-natural science

INTERNATIONAL MASTER'S PROGRAMMES
Applied Ethology and Biology,
Molecular Genetics and Physiology,
Ecology and The Environment
Materials Physics and Nanotechnology

DIRECTOR OF STUDIES
Agneta Johansson
Stefan Svensson
Ragnar Erlandsson
Leif Johansson/Magnus Johansson
Magnus Boman
Agneta Johansson
Agneta Johansson
Agneta Johansson
Leif Johansson/Magnus Johansson

GRADUATE TEACHING
IFM Graduate Programme
Per-Olof Holtz
Forum Scientium
Stefan Klintström
Agora Materiae
Per-Olof Holtz

RESEARCH DIVISIONS

SCIENTIFIC BRANCH OF APPLIED PHYSICS
Applied Optics
Hans Arwin, prof.
Stefan Klintström, Dr., chairperson
Applied Physics
Annita Lloyd-Spetz, prof.
Biomedical and Organic Electronics
Olle Inganäs, prof.
Biosensor and Bioelectronics
Anthony Turner, prof.
Biotechnology
Carl-Fredrik Mandenius, prof.
Molecular Surface Physics and Nanoscience
Kajsa Uvdal, prof.
Molecular Physics
Bo Liedberg, prof.
Surface Physics and Chemistry
/Thomas Ederth, assoc.prof., acting head of division
Mats Fahlman, prof.

SCIENTIFIC BRANCH OF BIOLOGY
Per Jensen, prof., chairperson
Ecology
Per Milberg, prof.
Molecular genetics
Johan Edqvist, assoc. prof.
Zoology
Jordi Altimiras, assoc. prof.

SCIENTIFIC BRANCH OF CHEMISTRY
Uno Carlsson, prof.
Biochemistry
Per-Olov Käll, prof.
Inorganic Chemistry
Bengt Harald Jonsson, prof., chairperson
Molecular Biotechnology
Roger Sävenhed, assoc. prof.
Organic Analytical Chemistry
Peter Konradsson, prof.
Organic Chemistry
Lars Ojamäe, prof.
Physical Chemistry
Per Hammarström, prof.
Protein Chemistry

SCIENTIFIC BRANCH OF MATERIAL PHYSICS
Weimin Chen, prof.
Functional Electronic Materials
Magnus Odén, prof.
Nanostructured Materials
Ulf Helmersson, prof.
Plasma & Coatings Physics
Erik Janzén, prof., deputy chairperson
Semiconductor Materials
Roger Uhrberg, prof.
Surface and Semiconductor Physics
Lars Hultman, prof., chairperson
Thin Film Physics

SCIENTIFIC BRANCH OF THEORY AND MODELLING
Bengt Persson, prof.
Bioinformatics
Sven Stafström, prof.
Computational Physics
Bo Ebenman, prof.
Theoretical Biology
Igor Abrikosov, prof., chairperson
Theoretical Physics
Financial Summary

OPERATING INCOME (AMOUNTS IN MSEK) 2012 2011
- University allocations for teaching 87 95
- University allocations for research 168 154
- External sources of income 193 170
  Total 448 420

OPERATING EXPENSES (AMOUNTS IN MSEK)
Expences for staff 237 222
Expences for premises 69 62
Other operating expenses 116 106
Depreciation 26 17
Total 448 407

Change in capital for the year 1 13
Balanced capital January 65 56
Balanced capital December 66 69

EXTERNAL SOURCES OF INCOME 2012 (AMOUNTS IN MSEK) 2012 2011
- Swedish Research Council, VR 54 57
- Other Research-funding agencies, e.g. Vinnova, Formas 18 19
- Research foundations, e.g. SSF 20 22
- Other private foundations, e.g. Wallenberg 30 15
- Funding from the European Union 32 22
- Other sources of funding 26 30
- Contract research 14 5
Total 193 170
Personnel Situation 2012

IFM STAFF JUNE 2012

<table>
<thead>
<tr>
<th>Position</th>
<th>Men</th>
<th>Women</th>
<th>Total</th>
</tr>
</thead>
<tbody>
<tr>
<td>Professors</td>
<td>46</td>
<td>9</td>
<td>55</td>
</tr>
<tr>
<td>Adj. Professors</td>
<td>4</td>
<td>0</td>
<td>4</td>
</tr>
<tr>
<td>Guest Professors</td>
<td>6</td>
<td>0</td>
<td>6</td>
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<tr>
<td>Senior Lecturers</td>
<td>42</td>
<td>18</td>
<td>60</td>
</tr>
<tr>
<td>Adj. Lectures</td>
<td>2</td>
<td>1</td>
<td>3</td>
</tr>
<tr>
<td>Assistant Lecturers</td>
<td>2</td>
<td>3</td>
<td>5</td>
</tr>
<tr>
<td>Researchers</td>
<td>3</td>
<td>0</td>
<td>3</td>
</tr>
<tr>
<td>Assistant Professors</td>
<td>22</td>
<td>6</td>
<td>28</td>
</tr>
<tr>
<td>Postdoctors</td>
<td>40</td>
<td>15</td>
<td>55</td>
</tr>
<tr>
<td>Other researchers</td>
<td>27</td>
<td>9</td>
<td>36</td>
</tr>
<tr>
<td>PhD students</td>
<td>81</td>
<td>48</td>
<td>129</td>
</tr>
<tr>
<td>Administrators</td>
<td>3</td>
<td>24</td>
<td>27</td>
</tr>
<tr>
<td>Engineers</td>
<td>21</td>
<td>4</td>
<td>25</td>
</tr>
<tr>
<td>Coordinator/Environment</td>
<td>0</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td><strong>Total</strong></td>
<td>299</td>
<td>138</td>
<td>437</td>
</tr>
</tbody>
</table>

NEW EMPLOYMENTS DURING 2012

<table>
<thead>
<tr>
<th>Personnel category</th>
<th>Men</th>
<th>Women</th>
<th>Total</th>
</tr>
</thead>
<tbody>
<tr>
<td>Senior Lecturers</td>
<td>1</td>
<td>1</td>
<td>2</td>
</tr>
<tr>
<td>Postdoctors</td>
<td>8</td>
<td>1</td>
<td>9</td>
</tr>
<tr>
<td>Other researchers</td>
<td>5</td>
<td>1</td>
<td>6</td>
</tr>
<tr>
<td>PhD students</td>
<td>7</td>
<td>0</td>
<td>7</td>
</tr>
<tr>
<td>Administrators</td>
<td>0</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td><strong>Total</strong></td>
<td>21</td>
<td>4</td>
<td>25</td>
</tr>
</tbody>
</table>

During 2012, 25 persons began their employment at the department.
New Professors 2012

NGUYEN TIEN SON, professor in Semiconductor Materials, received his PhD in solid state physics at the Department of Physics and Astronomy, University of Amsterdam in 1993. After that he worked as a postdoctoral fellow (1993-1997) at the division of Semiconductor Materials, IFM, Linköping University. He became docent (1999) and associate professor (2003) in materials science at IFM. His research covers from the fundamental properties of semiconductors to the physics of defects and the influence of defects on the material properties. The materials of interest include bulk Si, SiC, GaN, AlN, and ZnO as well as the thin-film structures of III-nitride alloys. In the research, different optical, electrical and magnetic experimental techniques, such as photoluminescence, deep level transient spectroscopy, magnetic and cyclotron resonance, have been employed. His current research interests focus on defect physics and defect engineering in SiC and III-nitrides (GaN, AlGaN and AlN) to solve material problems for their applications in high-power and high-frequency electronics and deep-ultraviolet light-emitting devices.

SERGEI SIMAK Doctor of Physical and Mathematical Sciences (2000) at National University of Science and Technology (MISiS), Moscow, Russia. Forskarassistent at The Department of Applied Physics, Chalmers University of Technology and Göteborg University, Gothenburg, Sweden 2000-2002. Forskare at The Department of Physics, Uppsala University, Sweden (2002-2004), University lecturer at IFM, Linköping University since 2004.

Sergei’s research is focused on studies of physical properties of materials based on fundamental laws of Nature, first of all the principles of Quantum Mechanics. What he does, can be described as “theoretical experiments” employing modern supercomputers instead of standard experimental equipment. He develops new methods which allow one to calculate and predict physical properties of solid materials at given external conditions, such as, for example, pressure, temperature and composition. In particular, he is deeply involved in studies of the Earth’s core and superhard materials. The results of his research are presented in many publications, in particular in high-impact journals Science, The Physical Review Letters and Proceedings of the National Academy of Science of the USA (PNAS).

Sergei’s main current interest is in the materials for fuel cells, i.e. the possible future sources of “green” energy which do not pollute the environment. His ultimate goal is theoretical materials design of fuel cells with optimum properties. This work brought substantial attention of the international scientific community. In particular, Sergei got a patent for the solid oxide fuel cell electrolyte, designed exclusively on the basis of quantum mechanical calculations. Excellent properties of the predicted material were later confirmed by experimentalists in Florida University, USA.


Sergei’s scientific interests would be incomplete without teaching. He is a teacher and developer of undergraduate and Ph.D. courses. In particular, he gives regular courses in Solid State Physics and Relativistic Quantum Mechanics at Linköping University. His international PhD courses “Quantum Simulation of Liquids and Solids” hosted by Centre européen de calcul atomique et moléculaire (CECAM) were great success and attracted young researchers from all over Europe. He has also been principal supervisor of 2 Ph.D students (both received the Ph.D. degree), 4 M. Sc. Students, and 2 Post. Docs.
The Environment

LEGISLATION
IFM has an injunction, according to the Swedish Environmental Code, to submit a yearly report to the local environmental agency describing the laboratory work at the department. The agency makes regular inspections at IFM.

ENVIRONMENTAL MANAGEMENT SYSTEMS
The Rector at LiU decided in 2006 that all departments must work according to an environmental management system. Since 2009 a regulation of environmental management for government agencies stipulates how to perform the environmental work. In 2010 an environmental enquiry was performed at LiU and resulted in several environmental target areas and goals.

At IFM a plan for the environmental work was first established in 2004 and resulted in measures taken towards reaching an environmental management system. An environmental plan for 2011-2012 was decided by the IFM board in March 2011 and consists of an action plan with environmental targets and measures needed to be taken. The environmental work has been presented in the local co-operation group during the year.

IFMS ENVIRONMENTAL TARGETS 2011-2012
The targets are organised according to the long-term environmental areas adopted by LiU and IFM and are to be accomplished by 2012-12-31.

LIMIT THE CONTRIBUTION TO THE CLIMATE CHANGES
1. Decrease the energy consumption of IT-equipment by installing energy-saving mode and increasing the number of switched off equipment.

A system for automatic measurements of the number of computers turned on or off was to be developed and implemented during 2012, but unfortunately it proved to be difficult to find a method that provided reliable data. When installing computers in offices etc., the computer support group always configures to energy-save mode. The measures to achieve the target were partly fulfilled.

2. Work shall be performed to take the previously designed measures to reduce the environmental impact from travel made by IFM.

Information to the IFM employees regarding the guidelines for environmentally friendly travelling set by LiU is needed during 2013. During 2012 it became possible to use the LiU card when travelling with the Campus bus. The measures to achieve the target were partly fulfilled.

3. IFM shall, whenever possible, buy computers with good environmental performance (use of electricity and content of hazardous substances) based on the demands in procurements of local/public framework agreements.

IFM follows the available framework agreement. The measures to achieve the target were fulfilled.

EFFICIENT USE OF NATURAL RESOURCES
4. IFM shall supplement the waste sorting system in accordance with decisions made by LiU regarding waste sorting.

The waste sorting system has been supplemented during 2011 and 2012; the measures to achieve the target were fulfilled.

MINIMAL IMPACT FROM USE OF HAZARDOUS OR CONTAGIOUS SUBSTANCES
5. IFM shall implement future guidelines for handling of hazardous waste and other laboratory waste at LiU.

IFM has decided to offer some of the most common containers for laboratory waste for free. Information regarding this and the new routine for laboratory waste was sent by e-mail and published at the IFM website. Information has also been given at different meetings during 2012. At IFM, the laboratories have embraced the new routines to a large extent. Information about the new routine for handling hazardous waste was given by e-mail and information at different meetings. The routine was published on the IFM website. The measures to achieve the target were partly fulfilled.

6. Risk assessments shall be made before all new experiments/laboratory work and when purchasing new equipment.

In the autumn 2012 LiU initiated work to improve information on the website, templates etc. When that work is completed, spring 2013, IFM employees will receive information about risk assessment. The measures to achieve the target were partly fulfilled.

ORGANIZATIONAL ACTION
7. At IFM all laboratories where work that can be considered risky takes place, must have an appointed person responsible for supervision of the laboratory.

Improvement is needed to make sure persons responsible for supervision of laboratories have a written delegation. Information was given at different meetings during 2012 and the work will continue during 2013. Laboratories at IFM have, to a large extent, a notice outside the entrance with contact information. The measures to achieve the target were partly fulfilled.
Equal Opportunities

IFM believes that equal opportunity is important for both students and employees. The institution has therefore assigned the responsibility of equal opportunity to a group with the following members: Lejla Kronbäck (administrative personnel), Anna Sundin (administrative personnel), Simona Eles (technical staff), Ulf Frykman (technical staff), Göran Hansson (prefect), Agneta Johansson (director of studies), Uno Wennergren (professor), and Linnéa Selegård (PhD student).

The group aims to meet once a month to discuss ongoing projects and initiate new ones. These projects are in some way related to one or several of the five main issues that we build our work around: gender equality and gender issues, ethnicity and religion or other belief systems, disability, sexual orientation and gender identity and victimization, discrimination and harassment at an individual level.

In order to prevent discrimination and harassment the group has drawn up an Equal Opportunity Strategy. We believe that this strategy will contribute to the following:

- an attractive study and work environment
- development and creativity
- quality in education and research
- equitable structures and processes

The Equal Opportunities vision

- IFM aims to be a study and working environment that makes full use of the resources contributed to the department by students and employees with different backgrounds, life situations and skills.
- IFM seeks to promote equal opportunities in the academic world and the community at large.
- Admission and recruitment processes should be non-discriminatory.
- IFM’s study programmes should formally offer equal opportunities and be accessible to, prepared for and considerate of the needs of various student categories.
- The content of IFM’s study programmes should promote equal opportunities as far as possible.
- New students should be received in such a way that they all feel welcome.
- Equal opportunities should prevail in terms of employees’ working conditions, salaries, influence, career prospects and scope for combining a professional career with responsibility for home and family.
- IFM seeks to make it easier for employees and students, irrespective of gender, to combine their studies with parental responsibilities.
- IFM aims to be free from all discrimination and harassment.

Projects we worked with during 2012

The equal opportunity group has worked with several projects during 2012 and listed below are some of the actions taken by the group:

Our website is continuously being updated with new information about our work. There are links to the university central equal opportunity group with related information found in both Swedish and English.

The personnel department ensured that there were no unjustified differences in salaries between men and women.

We are trying to achieve a distribution according to gender that is within 40%-60% in the Board of Directors and all other working groups at IFM.

We are continuously trying to increase the number of female guest lecturers and our goal is to have both genders within a range of 40%-60%.
The third university task

School contacts
Our department has always been very active in different forms of school contacts. For several years we have had young researchers part time employed for external contacts, one each from physics, chemistry and biology. IFM is represented in the board for school contacts of LiTH. The goal of this board is to coordinate and support existing activities, as well as developing new exciting activities.

Perhaps the most frequent activity is various study visits by children, young people and teachers. In May we have a popular activity directed to secondary and upper secondary school teachers, the May Mingle, Majminglingen. Schoolteachers and university teachers meet in lectures and discussions. This activity is arranged in cooperation with the Mathematics department.

Popular science week
In October we participated in a Popular Science week for the general public. This event was initiated by the Professor Per Jensen in 2005, and the interest is growing. The success of the initial Popular Science day has led to a larger three-day arrangement in cooperation with other departments, the Popular Science week. IFM participated with various exhibitions and lectures.

Open house days
Linköping University arrange yearly two open house days for schoolteachers and pupils, and IFM participated with hands-on exhibitions during these days.

Quintek
IFM received about one hundred female high-school students within the Quintek program, aimed to promote the interest for science and technology among the young women. At this event have the high-school students a chance to familiarize themselves with university studies though meeting university teachers, PhD-students and MSc-students from IFM in activities such as mini lectures, science demonstrations and general discussions.

Senior researchers and PhD students from the Semiconductor materials Division shared their excitement about science and research with the pupils from Katedralskolan. In an introductory lecture by Vanya Darakchieva and Olle Kordina, the youngsters learned about the properties and societal impact of group-III nitrides, graphene and SiC. The young people also visited key labs and witnessed growth runs and exciting experiments on materials characterization.
Education for Undergraduate Students

The undergraduate education given by the Department of Physics, Chemistry and Biology (IFM) had four main divisions 2012.

• Physics (Directors of Studies: Leif Johansson/Magnus Johansson)
• Physics - Measurement Technology (Director of Studies: Magnus Boman)
• Biology at the Natural science, Teachers and Engineering programs (Director of Studies: Agneta Johansson)
• Chemistry at the Natural science, Teachers and Engineering programs (Director of Studies: Stefan Svensson)

These divisions have in turn subprograms.

Physics

STAFF
• Directors of studies: Leif Johansson / Magnus Johansson
• Administrative assistants: Agne Virsilaitė Maras / Karin Bogg
• Technical staff: Hasan Dzuho and Jonas Wissting
• Teachers (with course responsibility): Torun Berlind, Jens Birch, Magnus Boman, Irina Buyanova, Valeriu Chirita, Per Eklund, Fredrik Eriksson, Jens Eriksson, Mats Eriksson, Ragnar Erlandsson, Urban Forsberg, Carl Hemmingsson, Lars Hultman, Magnus Johansson, Kenneth Järrendahl, Fredrik Karlsson, Peter Münger, Son Tien Nguyen, Wei-Xin Ni, Weine Olovsson, Plamen Paskov, Johanna Rosén, Per Sandström, Kostas Sarakinos, Bo Sernelius, Daniel Söderström, Roger Uhrberg, Chariya Virojanadara, Irina Yakimenko, Fengling Zhang

In our division, we are responsible for physics courses on the following 9 Engineering M.Sc. programs offered by the Institute of Technology at Linköping University. (The Swedish name of the degree from one of these programs is “Civilingenjör”.) A total of about 700 students are annually accepted in these programs.

D: Computer Science and Engineering (90)
I: Industrial Engineering and Management (180)
II: Industrial engineering and Management - International (40)
IT: Information Technology (30)
M: Mechanical Engineering (120)
MED: Biomedical Engineering (30)
MT: Media Technology and Engineering (60)
TB: Engineering Biology (30)
Y: Applied Physics and Electrical Engineering (90)
YI: Applied Physics and Electrical Engineering - International (20)

The nominal time for the Engineering M.Sc. programs is 5 years. The first three years mainly consist of compulsory courses in basic subjects and corresponds to B.Sc. degree. During the third year the students make a choice among the different specialisations (profiles) in years 4-5, which contain some compulsory courses (profile courses) but most are selectable and can be composed to fit the students own interest.

The Y(Yi)-students can choose between u profiles, two of which are related to our division:
• Theory, modelling and visualization (Irina Yakimenko)
• Material and nano physics (Jens Birch)

In addition, we also give physics courses on the Programme in Physics and Nanoscience (FyN), leading to a Bachelor of Science (3 years) with a major in Physics, and on the Master’s Programmes in Physics and Nanoscience (MFYS), Materials Physics and Nanotechnology (MPN), and Biomedical Engineering (BME).

Below is a list of the courses given by our division in 2012.

TUITION IN PHYSICS

Basic courses:
• Electromagnetic Field Theory (FyN, Y, Yi), 8hp
• Electromagnetism (summer course), 2hp
• Electromagnetism - Theory and Applications (IT, MED), 6hp
• Engineering Mechanics (D), 6hp
• Engineering project (MED, Y, Yi), 6hp
• Models in Physics (IT), 8hp
• Modern Physics (FyN), 8hp
• Modern Physics (MED, Y, Yi), 6hp
• Nano Scientific Project (FyN), 6hp
• Nanotechnology (BME, FyN, MFYS, MPN, TB, Y, Yi), 6hp
• Principles of Physics and introduction to Nanophysics (FyN), 10 hp
• Perspectives on Physics (D, FyN, Y, Yi), 2hp
• Physics (D), 6hp
• Physics (I, II), 6hp
• Physics (M), 8hp
• Physics of Sound (MT), 6hp
• Science and Technology for Renewable Energy Related Applications (FyN, MFYS, Y), 6hp
• Thermodynamics and Statistical Mechanics (FyN, Y, Yi), 6hp
• Wave Motion (FyN), 6hp
• Wave Motion (MED), 8hp
• Wave Motion (Y, Yi), 8hp
Advanced courses:
- Advanced Project Work in Applied Physics, 6 hp
- Analytical Mechanics, 6 hp
- Analytical Methods in Materials Science, 6 hp
- Chaos and Non-Linear Phenomena, 6 hp
- Classical Electrodynamics, 6 hp
- Computational Physics, 6 hp
- Elementary Particle Physics, 6 hp
- Experimental Physics, 6 hp
- Mathematical Methods of Physics, 6 hp
- Nano Physics, 6 hp
- Optoelectronics, 6 hp
- Physical Metallurgy, 6 hp
- Physics of Condensed Matter I, 6 hp
- Physics of Condensed Matter II, 6 hp
- Project course in Computational Physics CDIO, 12 hp
- Project Course in Physics - Design and Fabrication of Sensor Chip, CDIO, 12 hp
- Quantum Computers, 6 hp
- Quantum Dynamics, 6 hp
- Quantum Mechanics, 6 hp
- Semiconductor Physics, 6 hp
- Semiconductor Technology, 6 hp
- Surface Physics, 6 hp
- Thin Film Physics, 6 hp

Biology

STAFF
- Director of studies: Agneta Johansson
- Education secretary: Jessica Lövdahl and Eva-Maria Stigsdotter
- Engineers: Ingevald Abrahamsson and Tove Bjerg
- Teachers: Jordi Altimiras, Mats Amundin, Karl-Olof Bergman, Kjell Carlsson, Bo Ebenman, Johan Edqvist, Anders Hargely, Per Jensen, Matthias Laska, Ronny Lock, Örjan Lönnevik, Eva Mattsson, Per Milberg, Bengt Persson, Lina Roth, Karin S Tonderski, Corelia Spetea-Wiklund, Uno Wennnergren and Thomas Östholm

Courses in biology are offered as parts of the following study programmes:
- Biology Programme
- Bachelor of Science in Biology, profiles in Ecology, Environmental Management and Nature Conservation, Ethology and Animal Biology and Molecular Genetics and Physiology
- Masters of Science in Biology, profiles, Applied Ethology and Animal Biology, Ecology and the Environment and Molecular Genetics and Physiology
- Chemical Biology
- Engineering Biology
- The Program for education in Linköping
- Separate courses
- Basic year

THE BIOLOGY PROGRAMME, leading to the degree of Master of Science (240 credit points/hp) or to the degree of Bachelor of Science (180 credit points/hp). The programme includes, in the first two years, basic courses in chemistry and general biology. In the third and fourth years there are a number of advanced level courses, mainly seven profiles; Ecology, Ethology, Microbiology and Molecular Genetics, Conservation Biology, Theoretical Ecology, Zoology and Zoophysiology and Biomedicine and Cellbiology. The latter profile is carried out in collaboration with the department of Pharmacology and others within the Faculty

BACHELOR OF SCIENCE IN BIOLOGY, profiles in Ecology, Environmental Management and Nature Conservation, Ethology and Animal Biology and Molecular Genetics and Physiology (180 credit points/hp). The Programmes include, in the first two years, basic courses in chemistry and general biology. In the third year here are courses specific for each profile.

MASTER OF SCIENCE IN BIOLOGY, profile in Applied Ethology and Animal Biology, Ecology and the Environment and Molecular Genetics and Physiology (120 credit points/hp). The profiles in Applied Ethology and Physiology are a collaboration between the department of biology at Linköping University and the Kolmården Djpark.

The first year includes nine courses and at the end of the year the student start with his/her Master thesis. The Master thesis is a full year project that will take most of the second year. At the end of the second year the programme ends with a final course – Communicating science.

THE PROGRAMME FOR BIOLOGY AND CHEMISTRY WITH MATHEMATICS, leading to the degree of Master of Science (240 credit points/hp), or to the degree of Bachelor of Science (180 credit points/hp). After study of mathematics (40 credits) the student makes a choice of further studies in biology or chemistry.

THE CURRENT PROGRAM FOR EDUCATION for the Upper Secondary School and the Primary School started in 2001. The program involves a Biology and a Natur Science profile. The division has been responsible for the biology part of the program.

Biology courses are also given in the program CHEMICAL BIOLOGY (240 or 300 credit points/hp) and ENGINEERING BIOLOGY (300 credit points/hp).

SEPARATE COURSES. All courses within the Biology programme are also available as separate courses. Besides the courses in the Biology programme 8 separate courses has been given.

BACHELOR PROGRAMME, BIOLOGY PROGRAMME
- Animal Husbandry and its Administration, 6 hp
- Botany 1, 6 hp
- Botany 2, 6 hp
- Cell Biology, 6 hp.
- Degree Project - Bachelor’s Thesis, 16 hp
- Ecology, second course, 15 hp
- Ecology, 6 hp
- Environmental Management, 6 hp
- Ethology and Animal Welfare, 15 hp
- Environmental Engineering for Biologists, 15 hp
- Evolution, 6 hp
• Genetics, 6 hp
• Genomics and Bioinformatics, 9 hp
• Human and Animal Physiology: a problem based approach, 15 hp
• Introduction to Biology, 3 hp
• Introduction to Molecular Genetics, 6 hp
• Introduction to Scientific Methods, Analysis and Statistics, 6 hp
• Microbiology, 6 hp
• Molecular Biology, 15 hp
• Nature Conservation in Practise, 15 hp
• Principals in Physiology, 6 hp
• Zoology, Physiology, Morphology and Systematics, 6 hp

The Programme for Biology and Chemistry with Mathematics
• Animal Husbandry and its Administration, 6hp
• Ecology, second course, 15 hp
• Environmental Engineering for Biologists, 15 hp
• Environmental Management, 6hp
• Evolution 6 hp
• Final thesis, 30 hp
• Genomics and Bioinformatics, 9 hp
• Nature Conservation in Practise, 15 hp
• Population Ecology: Theories and Applications, 12 hp

Master of Science in Biology, profile Molecular Genetics and Physiology
• Adaption: Molecules to Organism, 6 hp
• Communicating science, 6 hp
• Current Concepts, 6 hp
• Degree Project - Master’s Thesis, 60 hp
• Functional Genomics, 6 hp
• Gene Expression Analysis, 6 hp
• Immunological Techniques, 6 hp
• Molecular Physiology, 6 hp
• Plant Molecular Genetics, 6 hp

Masters of Science in Biology, profile Ecology and the Environment
• Advancements in Ecology and the Environment - Part I, 6 hp
• Advancements in Ecology and the Environment - Part II, 6 hp
• Communicating science, 6 hp
• Conservation Biology in situ, 6 hp
• Current Concepts, 6 hp
• Degree Project - Master’s Thesis, 60 hp
• Methods in ecology, 6 hp
• Modelling of Biological Systems, 6 hp
• Population Ecology: Theories and Applications, 12 hp

Masters of Science in Biology, profile Applied Ethology and Animal Biology
• Adaption: Molecules to Organism, 6 hp
• Behavioral Neurobiology, 6 hp
• Communicating science, 6 hp
• Conservation Biology in situ, 6 hp
• Current Concepts, 6 hp
• Degree Project - Master’s Thesis, 60 hp
• Methods of Applied Ethology, 6 hp
• Primate Ethology, 6 hp
• Theory of Applied Ethology, 6 hp
• Zoo Biology, 6 hp

Programme For Education - Biology courses
• Biologi: Genetics, Botany, 15 hp
• Biology (ae 21-30), 15 hp
• Biology : Zoology, Physiology, Morphology and Systematics, 15 hp
• Biology: Cell Biology and Microbiology (ae 1-10), 15 hp
• Evolution and Applied Ethology (41-50), 15 hp
• Environmental Science & Introduction to Molecular Genetics (51-60), 15 hp

Engineering Biology
• Bioinformatics - Overview and Practical Applications, 6 hp
• Cell Biology, 6 hp
• Microbiology, 6 hp
• Principals in Physiology, 6 hp

Chemical Biology
• Behavioral Neurobiology, 6 hp
• Bioinformatics, 3 hp
• Bioinformatics - Overview and Practical Applications, 6 hp
• Cell Biology, 6 hp
• Genetics, 6 hp
• Immunological Techniques, 6 hp
• Microbiology, 6 hp
• Molecular biology, 15 hp
• Molecular Physiology, 6 hp
• Plant molecular genetics, 6 hp
• Principals in Physiology, 6 hp

Separate Courses
• Animal Behaviour, 15 hp
• Animal Communication II, 7,5hp
• Behaviour and Biology of the Dog, part 1, 7,5 hp
• Behaviour and Biology of the Dog, part 2, 7,5 hp
• Behaviour and Biology of the Dog, part 3, 7,5 hp
• Introduction to Ethology, 7,5 hp
• Faunistics & Floristics, 9hp, summer course
• Wetlands and Streams, Ecological Applications, 15 hp

BASIC YEAR
Biology for Foundation Year 3hp
Biology for Foundation Year 7,5hp

Chemistry

STAFF
• Director of studies: Stefan Svensson
• Education secretary: Rita Fantl
• Study counselor: Helena Herbertsson
• Technical staff: Bo Palmquist
Study programmes in Chemistry:

- Chemistry (Ke)
- Chemical Biology (KB)
- Chemical Analysis Engineering (KA)
- Master of Science program. Profiles: Organic Synthesis/Medicinal Chemistry and Protein Science
- Technical Biology (TB)
- Teacher Training Programs
- Separate Courses
- Basic Year

Most of the chemistry courses offered are part of the three-year programmes, **CHEMISTRY (Ke)** and **CHEMICAL BIOLOGY (KB)**, (180 credits points / hp). Students completing these programmes are awarded the degree of Bachelor of Science in Chemistry. All courses within the Chemistry Program are also available as separate courses.

The program, **CHEMICAL BIOLOGY (KB)**, have an open entrance for the students: after a year of studies the students can choose to continue in natural science (or to choose a more technical variant to become engineers. Chemical Biology combines understanding of complex biological processes with the fundamental principles of chemistry.

During 2009 all study programs were transformed into three-year Bachelor of Science programs (180 hp) and master programs on advanced level for further two years (120hp).

Chemistry offers master profiles in **ORGANIC SYNTHESIS/MEDICINAL CHEMISTRY AND PROTEIN SCIENCE**.

Some of the chemistry courses are also included in the study programmes of students majoring in **BIOLOGY** and in **TEACHER TRAINING PROGRAMS** (students becoming Upper Secondary School teachers). Biology bachelors are required to earn 21 hp chemistry, while Science Education majors earn up to 60-120 hp of chemistry. Introductory courses in chemistry for the study program **MEDICINAL BIOLOGY** were started under the autumn semester.

The above mentioned courses as part of the Mathematical Natural Science, chemistry courses are offered for engineering students in the M.Sc. program: **CHEMICAL BIOLOGY** (also mentioned above) and **ENGINEERING BIOLOGY (TB)** (270 hp).

**THE CHEMICAL ANALYSIS ENGINEERING (KA)** (180 hp), a three-year programme, has analytical chemistry as the main profile.

**BASIC YEAR** (130 students, 13 hp), with introductory courses in Chemistry on a secondary school level, is offered to students who do not meet the requirements for studies at the University.

Final theses, the last 30/45 or 60 hp in the Chemistry and Chemical Biology program, have been carried out by six students. For the engineering programs 14 KA students carried out the 16 hp, and 14 KB students the 30 hp final theses work in the chemistry area. Besides projects conducted on campus or at the University Hospital, were projects performed at different national companies and at University of Sidney.

Under the period 10 students were awarded the Master of Science degree and 17 students the Bachelor of Science from the Chemistry and Chemical Biology programs. From the Chemical Analysis Engineering program were 17 awarded the degree Bachelor of Science in Chemical Analysis Engineering and 15 Chemical Biology engineering students were awarded the M.Sc. degree.

Altogether approximately 600 students have enrolled in about 60 courses in chemistry through the year 2012.

<table>
<thead>
<tr>
<th>Courses</th>
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<td>General Chemistry 1</td>
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<td>Organic Chemistry 1</td>
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<td>Organic Chemistry</td>
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<td>Biochemistry 1</td>
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<td>Physical Chemistry - Thermodynamic</td>
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<tr>
<td>Analytical Chemistry S</td>
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<td>Organic Chemistry 2</td>
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<td>Analytical Chemistry T</td>
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<tr>
<td>Inorganic Chemistry</td>
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<td>Calculation Tools for Chemistry Students</td>
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<td>Experimental Chemistry</td>
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<td>Physical Chemistry - Spectroscopy</td>
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<td>Nano Chemistry: Surface and Colloid Chemistry</td>
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<td>Medicinal Natural Products</td>
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<td>Protein Chemistry</td>
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<td>Combinational Protein Engineering</td>
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<td>Biomolecular Design</td>
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<td>Degree Project - Bachelor’s Thesis (KB)</td>
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<td>Degree Project - Bachelor’s Thesis</td>
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<td>Degree Project - Master’s Thesis</td>
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<tr>
<td>Degree Project - Master’s Thesis (KB)</td>
<td>30/45/60</td>
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</tbody>
</table>

**TECHNICAL COURSES**

| Chemistry for Foundation Year | 7.5 + 6 |
| Organic Chemistry | 6 |
| Chemistry (C,Y,D) | 6 |
| Physical Chemistry (KB) | 6 |
| Analytical Chemistry (TB) | 6 |
| Biotechnical Biochemistry (I) | 6 |
| Life Scientific Research Review | 6 |
| Biostructural Technologies | 6 |
| Biochemistry 2 | 6 |
| Biological Measurements | 6 |
| Gene Technology | 3 |
| Project Course: Chemical Biology | 6 |
| Applied Structural Biology | 6 |
| Proteomics | 6 |
| Spectroscopy and Kinetics | 6 |
| Interactions and Recognition in Biomolecular Systems | 6 |
| Protein Engineering | 6 |
| Protein Chemistry | 6 |
| Environmental Chemistry | 6 |
| Biomolecular Disease Processes | 6 |
| Protein Engineering | 3 |
| Materials for Sustainable Energy Production | 6 |
| Fundamentals of Chemistry | 6 |
| Preparation of Proteins | 3 |
| Principles of Environmental Chemistry | 6 |
| Biochemistry 1 (KA) | 6 |
| Application Areas to Chemical Analysis Engineering | 6 |
| Introduction to Forensic Chemistry | 6 |
Physics – measurement technology

ACTIVITY FIELD
The division provides undergraduate courses in:

• Physics
• Measurement technology
• Biomaterials and Biotechnology

STAFF

• **Director of studies:** Magnus Boman.
• **Administrative assistants:** Karin Bogg, Rita Fantl, Åsa Forsell, Agne Virsilaitė Maras.
• **Technical staff:** Hasan Dzuho, Jonas Wissting.
• **Course leaders:** Daniel Alli, Mike Andersson, Valerio Beni, Peder Bergman, Lars Björklund, Caroline Brommesson, Thomas Ederyh Anders Elfswing, Lars Alfred Engström, Jens Eriksson, Mats Eriksson, Ragnar Erlandsson, Daniel Filippini, Anne Henry, Johan Hurtig, Olle Inganäs Henrik Jakobson, Magnus Johansson, Kenneth Järrendahl, Carl-Fredrik Mandenius, Weine Olovsson, Henrik Pedersen, Gáia Pozina, Mehrdad Rafat, Per Sandström, Anke Suska, Kajsa Uvdal

HIGHLIGHTS 2012

• The two separate divisions Physics, natural science and Measurement technology were merged into one common division: Physics – Measurement Technology.
• The new course Introduction to Biosensor Technology was developed (Valerio Beni).
• The new course Materials for Biomedical Engineering; from nano- to macro-level was developed (Caroline Brommesson).

PROGRAMMES
The courses are given for the:

• Engineering Master of Science programmes: BME, D, I, II, KB, M, MED, TB, Y.
• Engineering Bachelor of Science programmes: DI, EL, KA, MI.
• Bachelor of Science program: FyN.
• Programmes for Teacher Education: LÅR, ÅLP.
• Basic year and semester: BAS, BAST.
• and as Separate courses: FRI.

PROFILES
At an advanced level, courses are provided for two profiles:

• **Devices and Materials in Biomedicine (TB)**
  Profile leader: Karin Enander.
• **Industrial Biotechnology and Production**
  (KB, TB). Profile leader: Carl-Fredrik Mandenius.

COURSES

• Astronomy and Geophysics (FyN), 6 hp
• Basic education, physics (BAS), 15 hp
• Engineering Mechanics (KB, MED, TB), 6 hp
• Mechanics I (FyN), 6 hp
• Mechanics II (FyN), 4 hp
• Molecular Physics (TB), 6 hp
• Natural Science: Physics (LÅR, ÅLP), 15 hp
• Physics A (BAS), 7,5 hp
• Physics B (BAS), 12 hp
• Physics (KB, TB), 6 hp
• Physics 1-15 hp, (LÅR), 15 hp
• Physics 16-30 hp, (LÅR), 15 hp
• Physics 31-45 hp, (LÅR), 15 hp
• Physics 46-60 hp, (LÅR), 15 hp
• Physics 61-75 hp, (LÅR), 15 hp
• Planets, stars and galaxies (FRI), 4,5 hp
• Research at LiTH: IFM part
• Thesis in Physics (76-90 hp) (LÅR), 15 hp
• Wave Physics (EL, MI), 4hp

MEASUREMENT TECHNOLOGY:

• Computers in Measurement Systems (KA), 6 hp
• Contemporary Sensor Systems (BME, FyN, MFYS, Y), 6 hp
• Electrical Measurement Systems (EL), 4 hp
• Measurement Technology (FyN, Mat, MED, Y, Yi), 1,5 hp
• Measurement Technology (D, DI), 4 hp
• Measurement Technology (M, MI), 6 hp
• Measurement Technology (TB), 6 hp

BIOMATERIALS AND BIOTECHNOLOGY:

• Biomedical Materials (BME, TB), 6 hp
• Biosensor Technology (I, ii, KB, TB), 6 hp
• Biotechnology Manufacturing (KB, TB), 6 hp
• Biotechnology Project (I, ii), 6 hp
• Degree project - Master’s Thesis (TB), 30 hp
• Design of Biotechnical Process and Production -systems, project Course (KB,TB), 6 hp.
• Engineering Project (TB, KA), 6 hp
• Materials and Nanotechnology (TB), 6 hp
• Materials for Biomedical Engineering; from-nano- to macro-level (MED), 8 hp
• Materials in Medicine, CDIO-Project (TB), 6 hp
• Microsystems and Nanobiology (TB, Y), 6 hp
• Imaging and ubiquitous biosensing (TB), 6 hp
• Industrial Biotechnology (KB, TB), 6 hp
• Introduction to Biosensor Technology (MED), 6 hp
• Supramolecular Chemistry (TB), 6 hp
• Surfaces and interfaces (KB, MED, TB), 6 hp
• Surface Science (KB, TB), 6 hp
International Master’s Programmes

APPLIED ETHOLOGY AND ANIMAL BIOLOGY
This program deals with animal behaviour and biology from an applications perspective. Central issues are the biology of stress and animal welfare, domestication effects on behaviour, physiology of behaviour and conservation biology.

The programme is taught in association with Kolmården Zoo which sometimes is the teaching venue. Learning rests on a mix of classroom lectures, seminars and hands-on projects involving studies of animals in captive environments. All over the world, problems associated with keeping animals in captivity require increased attention and knowledge.

After completed studies, the student should be well-acquainted with theories of animal behaviour and biology, and have a close understanding of the concepts of animal welfare and conservation. Examination requires the ability to plan, implement and present a scientific investigation in the subject framework of the programme.

More information http://cms.ifm.liu.se/biology/

MASTER’S PROGRAMME IN MOLECULAR GENETICS AND PHYSIOLOGY, 120 ECTS
This master’s programme focuses on eukaryotic molecular genetics and physiology, with particular emphasis on how this relates to both embryonic development and adult homeostasis.

The programme is divided into a first year of courses and a second year of work on a particular research project in a laboratory setting. The courses are taught using a multitude of formats, including regular lectures, practical laboratories and seminar discussions.

The laboratory classes will utilize powerful biological model systems such as Arabidopsis or chicken to illustrate modern concepts of molecular genetics and physiology. The thesis project during the second year (diploma work) will be conducted in a research laboratory at LiU or other university, in industry or the public sector.

During the first and second year, there will be a parallel seminar course in Current Concepts in Life Sciences, involving research articles and research lectures by invited speakers. During the second year, a parallel course in thesis writing and presentation techniques will be given.

More information http://cms.ifm.liu.se/biology/

MASTER’S PROGRAMME IN ECOLOGY AND THE ENVIRONMENT, 120 ECTS
Students will develop a critical scientific approach to ecology and an awareness of its role in society. The programme includes training in skills in experimental design and ecological field methodology, both in the classroom and during the individual project in the second year which can be linked to current research projects at the department – e.g. in grassland and weed ecology, ecology and Biogeochemistry of shallow waters or conservation biology. Alternatively the link can be to other universities or research institutes.

This master’s programme also emphasizes the need for, and use of, mathematical models and statistical analyses for addressing complex ecological problems. Such methods serve as powerful tools to e.g. identify crop management strategies for effective biological control, understand life-history strategies and the risk of population extinction in a variable environment, or evaluate the preservation status of nature reserves and the impact of management schemes.

The courses cover theories in population, community and systems ecology and how they relate to current environmental problems. Examples are methods in ecology, mathematical modelling of biological systems and conservation biology.

More information http://cms.ifm.liu.se/biology/

MASTER’S PROGRAMME IN PHYSICS AND NANOTECHNOLOGY
Aim and Organisation: The Master’s Programme in Materials Physics and Nanotechnology educates specialists in the area of physics of novel materials. The master students are prepared for university or industry careers in materials related research and development.

The programme covers a wide range of materials including materials used in semiconductor and nano-technology. opto-electronics, biotechnical applications (biocompatibility), chemical and bio-sensors, mechanical applications such as hardness and elasticity etc.

The programme comprises four semesters. The first autumn semester consists to a larger part of compulsory courses while the two following semesters contains mainly elective courses. The fourth semester is assigned to the Master’s thesis project.

The student can choose courses among essentially four elective profiles:

- Electronic Materials and Devices
- Surface and Nano Sciences
- Computational Physics
- Organic Electronics and Sensors

The master’s thesis should be based on high quality scientific research within the area of the profile chosen by the student. This work can be performed either at Linköping University or at other universities.

Information about this master’s programme can be found on the web page: http://www.liu.se/en/education/master/programmes/6MMPN/?l=en

PROGRESS
The programme started in 1996 and around ten students have since then joined the programme each year. This year when tuition fees were introduced the number dropped so only five students entered the programme. The study results of our International master’s students have overall been good. Several of them have produced very good results and have after receiving their MSci degree continued to a PhD degree at LI TH, KTH, CTH, LTH, KU and at universities abroad.
**Graduate Education**

**Forum Scientium**

**A MULTIDISCIPLINARY DOCTORAL PROGRAMME WITHIN BIOLOGY, CHEMISTRY, MEDICINE, PHYSICS AND TECHNOLOGY**

March 2012 Forum Scientium arranged a Reunion where former PhD students and supervisors met the current

Stefan Klintström (*programme director, director of studies*), Charlotte Immerstrand (*assistant director of studies*), Ingemar Lundström (*chairperson of the scientific advisory committee*), Anette Andersson (*administrator*)

IFM is the host for the doctoral programme Forum Scientium (www.liu.se/scientium).

Forum Scientium is a multidisciplinary programme and the doctoral students have backgrounds within biology, chemistry, medicine, physics and technology. The research projects are located at two faculties, Faculty of Health Science and the Faculty of Science and Engineering. Forum Scientium has financial support from the faculty, from the supervisors and from the Swedish Research Council.

The strategic objectives are “PhDs well prepared for their future careers through a structured doctoral programme which includes research of world class, and cooperation and multifaceted contacts with industry and society”.

During 2012, the doctoral programme Forum Scientium had around 60 PhD-students, and 8 PhD-dissertations were defended.

Since 2008, a special Forum Scientium Award exists. Forum Scientium PhDs can apply for an award providing 50% of the salary for a period of up to one year from the PhD-exam. The award aim at promoting the future career for the awardees, and to promote twinning among active Forum Scientium members. Most important is also that they should be of benefit for the active PhD-students. The awardees are called “Transformers” and during 2012 we had all together five transformers.

**OTHER ACTIVITIES DURING 2012:**
- Ten monthly meetings at Campus US and Valla
- Reunion March 2012
- Study visit to the Boston area May 2012
- Summer Conference August 2012
- Poster competition August 2012
- Yearly individual follow-up with each PhD-student
- Courses of high quality and much more that can be found in the Forum Scientium Yearly Report that is published at www.liu.se/scientium.

**Agora Materiae**

March 2012 Forum Scientium arranged a Reunion were former PhD students and supervisors met the current

AFM *Director*: Lars Hultman  
Graduate *School Head*: Per Olof Holtz  
Graduate *School Mentor*: Stefan Klintström  
Graduate *School Administrator*: Kirstin Kahl  
Agora *Student Council in end of 2012*:  
Martin Eriksson (Semiconductor Materials)  
Christopher Tholander (*Thin Film Physics, IFM*)  
Thomas Fransson (*Computational Physics, IFM*)  
Mattias Calmunger (*Engineering Materials, IEI*)  
Roger Magnusson (*Applied Optics, IFM*)  
Zia Ullah Khan (*Organic Electronics, ITN*)

Agora Materiae is a Graduate School for PhD students working in the research field of novel functional materials. The Agora Materiae Graduate School is dedicated to offer graduate studies in a true multi-disciplinary environment. Agora was started up in the beginning of 2012 and has got 40 members during its first year. Agora Materiae is hosted by IFM, but attracts PhD students from several departments such as ITN and IEI. Agora has financial support from AFM, which manages larger investments in research and infrastructure, based on the strategic support from the Swedish government for materials-science.

The PhD students can work in an environment, at the forefront within several research fields within materials science and the students are offered breadth and depth in scientific and didactic competence. A student council with five or six PhD students in the Agora graduate school acts as contact between the Agora members and the management of the graduate school. The student council is responsible for activities e.g. study visits, the home page, symposia and a summer conference.
The Agora Materiae members will benefit from:
- specific training courses offered to Agora Materiae members, but also to the extensive menu of PhD courses at IFM
- research at the international forefront, in an international atmosphere, offering a broad scientific and didactic competence
- a large number of experienced thesis advisors from various disciplines
- research programs of high industrial relevance
- extensive and advanced experimental techniques available on state-of-the-art equipment

Some important activities within the Agora Materiae Graduate School are:
- Seminar activity. Every fourth week, there is a joint PhD students seminar activity. Also invited speakers, often former PhD students, give seminars at these occasions.
- Common courses. Agora Materiae graduate school will arrange common courses. Can also be compulsory courses for the graduate school.
- Study visits: There are visits to research-intensive companies and/or academic departments arranged. Also study visits outside Sweden will take place.
- Summer conference: Every year, there will be a summer conference during approximately three days arranged, with activities like invited presentations, poster sessions.
- Progress reports. Together with the individual study plan, the progress plans three times a year are a follow-up of the progress in the PhD-students projects, planning of their research work with the purpose to improve the communication between the PhD-students and their supervisors.
- Yearly individual follow-up. Each PhD student in Agora will have a discussion with the graduate school director to discuss project, progress, time schedule, but also problems in the graduate program.

### IFM Graduate Programme

**Per Olof Holtz, Director of Graduate Studies**

The graduate program at IFM, Linköping University aims at a degree of Licentiate or Doctor of Technology or Philosophy for the PhD students. The requirements for the Licentiate / PhD exam consist of a course part, corresponding to 30/45 and 60/90 credit points (hp), and a doctoral/licentiate thesis. The nominal time for training to the Doctor degree is four years (full-time training) and for the Licentiate degree approximately half the time. The PhD students are encouraged to do teaching at undergraduate level (at maximum 20% of their time), which means that the total time to provide the Doctor degree can be up to five years. During the year 2012, 38 new students entered the graduate program at IFM with PhD as the final exam and 3 new students started the graduate program with the licentiate exam as the final exam. For a development of the number of students entering the graduate program at IFM during the last five years, see Diagram 1 below.

<table>
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<th>2008</th>
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Diagram 1 showing the number of students entering the graduate program at IFM during the last five years.

During the year 2012, there were in total 50 exams: 31 PhD exams and 19 licentiate exams, taken at IFM. For a development of the exams during the last five years, see Diagram 2 below.

<table>
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<td><strong>Total</strong></td>
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<td>3</td>
<td>9</td>
<td>19</td>
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</table>

Diagram 2 showing the number of exams from the graduate program at IFM during the last five years.

The course menu is organized jointly for the different scientific research groups at IFM, which means that a broad course menu within physics, chemistry and biology is offered, reflecting the strong inter-disciplinary character of IFM. During the academic year 2011/12, the PhD students could choose between approximately 60 courses at IFM. The students can also follow courses given at the graduate schools Agora Materiae and Forum Scientium at IFM, at other departments of Linköping University or at other universities. For all PhD students, who do teaching at undergraduate level, a basic pedagogics course is compulsory. IFM is arranging a specific pedagogics course for PhD students registered at the department. A course in science methodology and ethics is compulsory for all PhD students.

At IFM, a doctoral-studies board is a forum for various topics associated with the graduate studies. This council, with four meetings per year, has the following members: The Director of Graduate Studies, one representative for each scientific research area at IFM and two PhD student representatives from Physics and Chemistry/Biology, respectively.

Each graduate student has to make up an individual study plan each year. This study plan should contain a time schedule for the PhD studies, a project plan for the research work together with teaching and other duties at the department. This individual study plan is followed up each year.
PhD Courses Offered

DURING THE ACADEMIC YEAR 2011/12

• Introductory course in Scanning Probe Microscopy (3 hp): Ragnar Erlandsson
• Quantum Dynamics (6 hp): Irina Yakimenko
• Quantum computers (6 hp): Irina Yakimenko
• Quantum mechanics II (7.5 hp): Irina Yakimenko
• Electronic Structure Theory (5 hp): Igor Abrikosov
• Chemical Vapor Deposition (8 hp): Henrik Pedersen
• Ion Beam Analysis in Material Science (7.5 hp): Jens Jensen
• Soft Materials and Self Assembly: Niklas Solin
• Theoretical ecology – society related ecology (6 hp): Bo Ebenman
• Organic Chemistry (7.5 hp): Stefan Svensson/Peter Konradsson
• Differential equations for bio applications: Peter Munger/Bo Ebenman/Uno Wennergren
• Biotechnology, Advanced course (10 hp): Carl-Fredrik Mandenius
• Biotechnology Exp. Techniques (10 hp): Carl-Fredrik Mandenius
• Computational Quantum Chemistry (7.5 hp): Patrick Norman/Matieu Linares/Bo Durbeej
• Microsystems and nanobiology (6 hp): Anders Elfwing
• Molecular Mechanics and Dynamics in Chemistry: Matieu Linares
• Magnetic resonance characterization of defects in semiconductors (6 hp): Nguyen Son
• Chemical Sensor and Science Technology (4 hp): Anita Lloyd Spetz
• Contemporary Sensor Systems (6 hp): Anita Lloyd Spetz
• NEXAFS: Kajsa Uvdal / Patrick Norman
• Molecular imaging, vibrations: Thomas Edert
• Growth of wide bandgap semiconductors: Anelia Kakanakova
• Electrical characterization of semiconductor materials and devices: Einar Sveinbjörnsson
• Advanced methods for XRD (5 hp): Jens Birch
• Nano Physics (6 hp): Plamen Paskov
• Properties of III-nitride semiconductors (5 hp): Plamen Paskov
• Advanced semiconductor materials (7.5 hp): Vanya Darakhchieva
• Analytical Methods in Materials Science (AMMS) (6 hp): Fredrik Eriksson
• Many particle physics I (7.5 hp): Bo Sernelius
• Electrodynamics (6 hp): Bo Sernelius
• Surface Physics (6 hp): Chariya Vironjanadara
• Introduction to theoretical methods in material physics: Björn Alling
• Semiconductor physics (10 hp): Peder Bergman
• Time resolved spectroscopy: Galia Pozina / Peder Bergman
• Raman spectroscopy (3 hp): Ivan Ivanov
• Nucleation, growth and structural evolution of thin films and nano structures: J Greene / L Hultman / J Birch
• Statistical Methods in Experimental Sciences (4 hp): Anders Grimvall (HU)
• Basic management of Research Projects (1.5 hp): Stefan Klintström / Rune Olsson
• Bioethics/research ethics (3 hp): Stellan Welin / Health University
• Intellectual Properties as a Business Tool (3 hp): Stefan Klintström/Lena Sjöholm
• Magnus Kloftsen/Arne Jakobsson
• Modern Biology for non-biologists (6 hp): Stefan Klintström
• Biosensor Technology (6 hp): Fredrik Winquist
• Advanced Biosensor Technology with Medical Applications (4/6 hp) Fredrik Winquist
• Chemistry (6 hp): Nils-Ola Persson
• Biophysical Chemistry (7.5 hp): Nils-Ola Persson
• Nano Chemistry II (Surfaces and Colloids) (6 hp): Nils Ola Persson/Lars Ojamäe
• Introduction to Concepts in Molecular Genetics: Per Jensen
• Scientific Publishing (3 hp): Per Jensen
• Biomolecular interactions (7.5 hp): Anki Brorsson/Bengt-Harald Jonsson
• Bio/ nano technology (3hp): Bengt-Harald Jonsson
• Protein Chemistry: Lars Göran Märtensson / Maria Sunnerhagen
• Defects and dislocations: Jawad UU Hassan
• Fluorescence Microscopy: Per Hammarström
• Molecular Basis of Protein Conformational Diseases: Per Hammarström
• Semiconductor physics (6 hp): Fredrik Karlsson
• Imaging and Ubiquitous Biosensing (6 hp): Daniel Filippini
• Applied structure biology (6 hp): Maria Sunnerhagen
• Biomolecular structure analysis (6 hp): Patrik Lundström
• Bio measurement technology (6 hp): Maria Sunnerhagen
• Statistical and Thermal Physics I (7.5 hp): Peter Munger
• Transmission Electron Microscopy I (7.5 hp): Per Persson
• Vacuum science and technology (7.5 hp): Per Eklund
• Chaos and non-linear phenomena (6 hp): Magnus Johansson
• Semiconductor device physics (7.5/10 hp): WeiXin Ni
• Optoelectronics (6 hp): WeiXin Ni
• Thin film physics (6 hp): Ulf Helmersson
• Plasma physics (6 hp): Ulf Helmersson / Kostas Sarakinos
• Cluster Assembled materials (6 hp): Gueorgui K. Georgieiev
• Photovoltaic energy conversion: Koen Vandewal/Olle IngaNäs
SCIENTIFIC BRANCH OF
Applied Physics

General Information

STEERING COMMITTEE DURING YEAR 2012
Prof Bo Liedberg (chairperson Jan-March), prof Kenneth Järrendahl, prof Kajsa Uvdal, prof Olle Inganäs, prof Carl-Fredrik Mandenius, prof Anthony Turner, prof Anita Lloyd Spetz, prof Kajsa Uvdal and ass prof Stefan Klintström (chairperson April-Dec).

RESEARCH DIVISIONS AND PROFESSORS
Applied Optics: Kenneth Järrendahl, Hans Arwin
Applied Physics: Ragnar Erlandsson, Helen Dannetun (Rector Linköping University), Martin Holmberg (Guest Prof from Swedish National Defence College, Stockholm, Sweden), Pentti Tengvall (Guest Prof from Gothenburg University, Sweden)
Applied Sensor Science: Anita Lloyd Spetz
Biomolecular and Organic Electronics: Olle Inganäs
Biosensors and Bioelectronics: Anthony Turner, Fredrik Winquist, Ingemar Lundström (Emeritus)
Biotechnology: Carl Fredrik Mandenius, Anders Brundin (Adjunct)
Molecular Physics: Bo Liedberg
Molecular Surface Physics and Nanoscience: Kajsa Uvdal
Surface Physics and Chemistry: Mats Fahlman

LARGER RESEARCH PROGRAMMES
- Strategic Faculty Grant AFM – Advanced Functional Materials
- VINNEX Center FunMat
- The Linköping Center for Nanoscience and Nanotechnology - CeNano
- EU Marie Curie ITN “Seacoat”
- SSF funded OPEN (Organic Hybrid Printed Electronics and Nanoelectronics)
- A Cost Network, EuNetAir
- Linköping Initiative for Life Science Technologies (LIST)
- Power Papers funded by the Knut and Alice Wallenberg foundation
- EU Marie Curie ITN Renaissance
- EU Modelling of electronic processes at interfaces in organic-based electronic devices (MINOTOR)
- EU All-carbon platforms for highly efficient molecular wire-coupled dye-sensitized solar cells (MOLESOL)
- EU Next Generation Hybrid Interfaces for Spintronic Applications (HINTS)
- EU SUstainable Novel Flexible Organic Watts Efficiently Reliable (SUNFLOWER)

SUMMARY OF ACTIVITIES
The research within the Scientific Branch of Applied Physics is multidisciplinary and in many cases directed towards the area of Life Science Technologies.

There were 38 PhD students within the Scientific Area Applied Physics during 2012. Four PhD students did successfully defend their PhD thesis, and two defended their Licentiate.

Most of the PhD students participate in the graduate schools Forum Scientium or Agora Materiae (see separate entries). The PhD students work normally in projects that involve two or more divisions or departments at Linköping University. Forum Scientium is directed by Dr Stefan Klintström, who also is the chairperson of the Scientific Area Applied Physics.

EDUCATION
Staff from the Scientific Area Applied Physics teaches in several undergraduate programs, especially within the programmes “Engineering Biology” and “Applied Physics and Electrical Engineering”.

Highlights during 2012

WASTE MATERIALS FROM PAPER PULP PROCESSING TO BUILD POLYMER ELECTRODE FOR STORING CHARGE

Polymer electrodes incorporating polypyrrole and lignin derivatives, coming from brown liquor formed during paper processing, enable charge storage in the quinone functions deriving from lignin. [G. Milczarek and O. Inganäs, Science 335 (6075), 1468 (2012)]

NEW GENERATION SiC-FET GAS SENSORS
A new generation of SiC-FETs was developed by the spin-off company SenSiC AB in collaboration with Applied Sensor Science and FunMat. The new sensors show largely improved sensor characteristics in terms of selectivity, sensitivity and long-term stability. It is also possible to fine-tune the operation parameters for use of the sensors in alarm purposes, demonstrated for ammonia.

_LAYOUT OF SiC-FET GAS SENSOR CHIP INCLUDING SENSORS AND RESISTIVE HEATER. BACKGROUND, PART OF THE PROCESSED SiC WAFER._

 фон Лютен Спетц was appointed Deputy Chair of the COST Network, EuNetAir TD1105, with partners from 25 countries in the field of New Sensing Technologies for Air-Pollution Control and Environmental Sustainability.
SWEDEN-JAPAN SEMINAR ON NANOMATERIALS AND NANO-TECHNOLOGY (SJS-NANO)
The Sweden-Japan Seminar on Nanomaterials and Nanotechnology (SJS-Nano) was organized 10-11 September 2012 by Linköping Biosensors and Bioelectronics Centre, IFM, Linköping University. Sessions included theoretical and experimental works on:
- Biomedical Nanotechnology
- Nanotheragnostics
- Energy and Environmental Nanotechnology
- Nanobioanalytics
- Nanofabrication and Engineering

THE 22ND WORLD CONGRESS ON BIOSENSORS IN CANCÚN, MEXICO

Biosensors 2012 was held in Cancún, Mexico, from Tuesday 15 to Friday 18 May 2012. Congress Chairperson of the event was Prof Anthony P F Turner, Linköping University, Sweden.

Summer School on Printed Biosensors Organised by LIU in Cancún, Mexico
The pre-congress Summer School on Printed Biosensors and Electronics, aimed at providing an in depth and tutorial view of this specialist topic. This was organised by Linköping University in association with Elsevier and supported by Erkon. The increasing popularity of the Summer School was demonstrated by the capacity audience of around 100 delegates. The delegates were treated to a unique insight into the commercial reality of biosensor production with copious amounts of information being provided that does not appear in the conventional academic literature. This “how-to-really-do-it” day was extremely well received by the audience.

Workshop “Bioinspired Nanotechnologies for Distributed Diagnostics”
COST-LIST workshop 26/27 April 2012
The workshop was organised by the three organizations:
- COST Action TD1003 - Bio-inspired nanotechnologies: from concepts to applications
- LIST - Linköping Initiative in Life Science Technologies
- Hälsans nya verktyg - New tools for health

Linköping Initiative in Life Science Technologies (LIST) is an LIU Center, focused on the development of future health care solutions and an important contribution from LIU to the regional Vinnova supported program “New Tools for Health”. The missions of LIST are to stimulate the interest for and increase the possibilities to perform excellent research on new technologies for distributed health care at LIU and to reinforce the importance of long-term collaboration between faculties in this research area. The Scientific branch of Applied Physics is engaged in LIST through Karin Enander (part time director), Anke Suska (part time co-director), Ingemar Lundström (chairperson of the steering committee) and Anthony Turner (member of the steering committee).

LIST activities include support of research projects (in total 1 MSEK/year) and arrangement of workshops. In 2012, LIST granted financial support to the following projects:
- “Optically coupled touch screens for lab-on-a-chip medical diagnostics”; PI: Daniel Filippini (IFM).
- “Behavior analysis in elderly HF patients”; PIs: Pierangelo Dell’Acqua (ITN) and Tiny Jaarsma (ISV).
- “Wearable contact lens biosensors with nanoengineered architecture at interface”; PIs: Martin Mak and Ashutosh Tiwari (IFM).

In April 2012, LIST co-arranged the international LIST/COST symposium “Bioinspired nanotechnologies for distributed diagnostics” and in October, senior scientists from different faculties at LIU were invited to meet in a scientific speed-dating format with the purpose of forming new research collaborations. This event turned out to be very successful and will be followed by more arrangements of similar kind.

Royal Society of Chemistry Award Lecture Tour
Professor Turner was sponsored to present a series of Award lectures in the UK, Ireland and Italy during the spring of 2012 culminating in a ceremony at Imperial College, London, at which he was presented with the Royal Society of Chemistry Theophilus Redwood Medal for his outstanding contribution to Analytical Science.

A Tutorial Review based on the lectures will be published by the prestigious journal Chemical Society Reviews.
Applied Optics

STAFF
Professors: Hans Arwin, Kenneth Järrendahl, Arturo Mendoza Galván
Administrative assistant: Anna Maria Uhlin
Assist. professors: Sergiy Valyukh, Tomas Hallberg (external)
Post docs: Torun Berlind, Iryna Valyukh
PhD students: Lia Fernández del Río, Roger Magnusson, Eloy Muñoz Pineda, Christina Åkerlind
Visiting/diploma students: Rodrigo Becerra Carrillo, Eduardo de Mayolo, Johan Gustafson, Adam Icardi, Lia Fernández del Río, Kristofer Krus, Venkata Sai Dinesh Sugavasi, Sebastian Ekeroth


NATURAL PHOTONIC STRUCTURES Optical properties of cuticles of several beetles were studied to learn how nature has designed biomulilayers. Figure 1 show a specimen of Chrysisina gloriosa viewed through a left-polarizing (LPC) and right-polarizing (RPC) filter (Arwin, Fernández, Järrendahl, Landin, Magnusson).

The polarization properties of three specimens of Cotinis mutabilis with different color were studied by analyzing the Mueller matrix data and complemented with the structure revealed by microscopy techniques (Muñoz, Mendoza, Arwin, Järrendahl).

BRDF measurements and Mueller-matrix ellipsometry on Cyphochilus insulans was performed to analyze scattering and depolarization properties (Åkerlind, Hallberg, Arwin, Järrendahl).

ARTIFICIAL PHOTONIC STRUCTURES Gold-silica dot arrays were investigated in collaboration with M. Käll and a model describing their optical response was developed. Figure 2 show transmission data from this kind of structure (Mendoza, Järrendahl, Arwin). Nanostructured helical films composed of InAlN nanorods were fabricated and analyzed in collaboration with J. Birch at LIU. Left-handed and right-handed structures were grown. In collaboration with Ecole Polytechnique in Paris imaging Mueller-matrix analysis was performed (Magnusson, Arwin, Järrendahl).

ELECTROCHROMIC THIN FILMS Tungsten doped NiO films with different compositions were characterized by ellipsometry. Dielectric functions of nickel doped WO3 were studied in terms of the Bruggeman effective medium approximation. Inhomogeneous Au films with mass thickness from 1.5 to 10 nm on glass substrates were characterized by spectroscopic ellipsometry (I. Valyukh).

ACTIVE OPTICAL ELEMENTS Diffractive elements based on liquid crystals are studied with focus on non-uniform alignment conditions that enable us to achieve the needed distribution of the liquid crystal molecules under a uniform external electric field. (S. Valyukh). An objective LC micro-lens array for a display located at the immediate vicinity of the eye has been proposed. The developed micro-lens array changes optical power from 0 to up to 500 dioptres and is a promising technique for augmented reality. (S. Valyukh). Non-absorptive flat thin reflectors, based on cholesteric liquid crystal polymers, with specific spectral and spatial characteristics have been developed and patented. Among the areas of applications are optoelectronics and photovoltaics (S. Valyukh).

PROTEINS AND CELLS AT INTERFACES In collaboration with Håkan Engqvist, UU, (SSF Strategic Research Center, MS2E) surfaces aimed for bone replacements are examined. (T. Berlind).

CELLULOSE FILMS AND CHITIN FILMS In collaboration with Lars Wågberg, KTH, optical properties of cellulose films and humidity induced changes are studied with in situ spectroscopic ellipsometry.

The optical properties of dip-coated chitin thin films are also studied. Chitin is a semi-crystalline biopolymer found in the beetle’s cuticle as nanofibrils in a helical lamella structure which is responsible of the fascinating and complex polarization properties. In situ spectroscopic ellipsometry is used to study the changes induced in amorphous and semi-crystalline chitin thin films by humidity and temperature (Muñoz, Mendoza, Järrendahl, de Mayolo, Arwin).

SCIENTIFIC OUTPUT 2012 8 publications, and 24 conference contributions including 3 invited talks.

SPECIAL EVENT Sergiy Valyukh became docent (ass. Prof.). Applied Optics was represented at the exhibition NANO, at Norrköpings Visualisering-center showing polarizing scarab beetles.

TEACHING Järrendahl, Berlind, S. Valyukh and Arwin were responsible for many undergraduate courses and activities. Kenneth Järrendahl is vice chairman for the EF study board.
Applied Physics

STAFF
Professors: Ragnar Erlandsson, Helen Dannetun (Rector at Linköping University), Martin Holmberg (Guest Prof from Swedish National Defence College, Stockholm, Sweden) and Pentti Tengvall (Guest Prof from Gothenburg University, Sweden)
Associate professors: Mats Eriksson, Daniel Filippini
Assistant professor: Stefan Welin Klintström (head of the division)
Researcher: Dr Anke Suska
Administrative staff: Anna Maria Uhlin
PhD students: Roger Klingvall, Zafar Iqbal, Pakorn Preechaburana
Research engineers: Jörgen Bengtsson, Jeanette Nilsson, Hans Sundgren and Bo Thunér (lab manager)

GENERAL INFORMATION
The research within the Division of Applied Physics is multidisciplinary. The members of the division are electrical engineers, physicists, chemists, biochemists and biologists. Several projects are in the areas between physics and chemistry, and physics and biology. The projects are often conducted in collaboration with other divisions within the three scientific branches of Applied Physics, Material Science and Chemistry. The research activities also include fundamental multidisciplinary research, mainly within the surface sciences. Many projects are run in cooperation with external collaborators. The division is hosting Forum Scientium, a multidisciplinary doctoral student programme under the direction of Dr Stefan Klintström. See more under “Graduate education”. The division also participates in two VINNOVA-graduate schools: Forum Securitatis, a graduate school in security research and AgoraLink, an agora for Medical and Life Science Technologies in Linköping.

RESEARCH OVERVIEW, HIGHLIGHTS, AND COLLABORATIONS
The research within the Division is conducted in collaboration with many different parts of IFM and with larger programs described elsewhere. This means that some activities are more extensively described at other places in the Activity Report. The research groups within the Division of Applied Physics are led by:
• Ass prof Mats Eriksson
• Ass prof Daniel Filippini
• Dr Anke Suska

RESEARCH GROUP DANIEL FILIPPINI
OPTICAL DEVICES LAB
Daniel Filippini’s group works on optical chemical sensing methods and devices. One important area of the group’s activity is on physically interfacing chemical sensing techniques to operate on consumer electronic devices (CEDs). The other main research focus is microfabrication methods for disposable optics and fluidics. CEDs sensing ubiquity is restricted by the availability of the chemical sensing element and accessories rather than the CED platform itself. Hence, the critical requirements for cell phone applications are the development of chemical sensing inter-
faces deployable at a comparable scale and the formulation of solutions, which demand neither permanent modifications nor additional peripherals. Disposable lab-on-a-chip (LOC) devices can satisfy these requirements, if the measurement principle can accommodate the desired analytical performance. In 2012, Filippini’s groups demonstrated the first angle-resolved surface plasmon resonance (SPR) detection system that is based on a single disposable device, which is configured to use conditioned illumination and optical detection from cell phones. The SPR coupler central to this implementation is compatible with regular (LOC) technology and temporarily adheres to the phone screen surface during the measurement; it couples and conditions the illumination from the screen and directs the SPR image to the phone camera. After the measurement, the device can be detached and disposed of, thereby leaving the phone intact. SPR detection, within diagnostics range, was illustrated with a commercial assay for β2 microglobulin (β2M), which is an established marker for cancer, inflammatory disorders, and kidney disease, which are relevant candidates for complementary monitoring in decentralized conditions.

Biacore SPR chip evaluated with a smart phone aided by a disposable optical coupler. Sensorgram of label-free β2 microglobulin detection within the diagnostics range (P. Preechaburana, M. Collado Gonzalez, A. Suska, D. Filippini, Angewandte Chemie 51 (2012))

RESEARCH GROUP MATS ERIKSSON
S-SENCE
This is a research group within bio- and chemical sensor science and technology. Eriksson is also a member of the management group of Security Link, a strategic research area at LiU on technology and methodology for civil security applications. “Microelectrode arrays for drinking water quality monitoring” is an ongoing project financed by Formas and running 2011-2014. In this project new sensors with improved properties for drinking water monitoring, such as improved detection limits and faster response times, are developed. Several types of arrays are investigated as well as a new type of printed electronics microband structure (see figure), developed by the groups postdoc Mikhail Vagin together with Acreo.
**Biomolecular and organic electronics**

**STAFF**
- **Professor:** Olle Ingranäs
- **Associate professor:** Dengling Zhang, docent Niclas Solin
- **Visiting scientists:** Shimelis Admassie, Hongyu Zhen, Yizheng Liu
- **Postdocs:** Kristofer Tvingstedt (-July), Koen Vandewal(-Feb), Doddahalli Nagaraju, Shuyan Shao, Feng Gao (Feb), Wolfgang Tress (April), Mahiar Hamedi (-Aug), Deyu Tu
- **Graduate students:** Viktor Andersson(-Feb), Anders Elfving, Zaifei Ma, Fredrik Bäcklund, Zheng Tang, Jonas Bergqvist, Armantas Melianas (Sept-), Erica Zeglio (Nov-), Fatima Aijan (Dec-)

**Visiting students:** Yang Zhao, Armantas Melianas, Scott Mauger, Tomasz Rebis, Indre Urbanavičiūtė, Bedasa Abdisa, Sai Bai

**Administrators:** Mikael Amlé 65%,

**Research engineer:** Bo Thunér (27%)

**Diploma students:** Alexander Vastesson

**SUMMARY:**
Research in biomolecular and organic electronics is focused on the development of polymer electronics, particularly polymer photovoltaics, and the combination of biological macromolecules with synthetic conjugated polymers for supramolecular materials assembly. We published 14 papers during 2012.

**BIOMOLECULAR ELECTRONICS**

We published in Science the first generation of biopolymer-based polymer electrodes, where a electronic polymer is storing charge in a biopolymer which is modified to be electroactive. Further developments of polymer electrodes incorporating electroactive biopolymers has been done. By adding small quinone compounds into the biopolymer composites, considerable improvement of charge densities is obtained. These polymer electrodes are of relevance for energy storage in supercapacitors and possibly in secondary batteries based on aqueous electrolytes.

Decoration of DNA chains with metallic conjugated polyelectrolytes has been accomplished. Stretched and aligned decorated DNA chains acts as the conducting channel in a electrochemical transistor geometry, with sparsely printed wires connecting two electrode pads.

We have prepared self-assembled protein structures incorporating iron oxide nanoparticles. Moreover, these hybrid materials have been used as test systems in electron tomography measurements.

**PHOTOVOLTAICS**

We have evaluated the anisotropy of the charge transfer state, which is an intermediate state on the path to photocurrent in polymer/fullerene devices, through materials and device studies of oriented polymer systems.

Semi-transparent solar cells based on modified ITO cathodes combined with transparent polymer anodes have been developed. Stacking a number of these cells on top leads to a higher photocurrent than can be obtained by a standard geometry, where a reflective metal act both as cathode and mirror. With these semitransparent solar cells, we have also recouped some of the transmitted photons with the help of an external micropatterned metal reflector, which is superior compared to a flat metal mirror in improving the total amount of absorbed photons in the active device.

We investigated the effects of poly(ethylene oxide) (PEO) modified ZnO nanoparticles as electron acceptors in Hybrid Solar Cells. Compare with reference device using ZnO as electron acceptor, after PEO modification, all the device parameters are enhanced. Typically, the PCE was enhanced by 42% increase. When ZnO used as an interfacial layer between ITO and active layers in inverted OSCs, the best inverted solar cells were the ones based on the smoothest ZnO layers, with the largest D/A interfacial area, and lowest ZnO/active layer interfacial area.

We found that the performance of inverted OSCs can also be improved with PEO modified ZnO nanoparticles (NPs) as interfacial layers. PEO modified ZnO surface can effectively passivates the surface traps of ZnO, suppress the combination loss of carriers, reduce the series resistance, and improve the electrical coupling of ZnO/active layer. PCE could be increased from 4.4% to 5.7%.
TEACHING
Teaching in the undergraduate curriculum included the undergraduate courses Microsystems and nanobiology (TB), Materials and Nanotechnology (TB), Introduction to renewable energy and energy saving.


Collaborations: With Chalmers University for polymer materials, and with Lund for spectroscopy. With Björn Högberg, Karolinska Institutet for DNA origami. With Beijing Normal University, China, Zhejiang University, China, Georgia Institute of Technology, US and ISE, Freiburg, Germany.

Funding in the field of printed organic electronics and organic nanoelectronics comes from SSF, through the program OPEN 2008-2013. The Wallenberg Scholar fund for Olle Inganäs has been instrumental in creating novelty, and the Wallenberg foundation funded project Power Papers, together with Magnus Berggren at ITN will consolidate these new topics.

We held a Swedish-Sino bilateral workshop on polymer photovoltaics, 31/10-1/11, 2012, IFM, LiU.

We organized the national MicroSystem Workshop (MSW-2012) in May 2012, with ≈ 100 participants.

HIGHLIGHTS

Polymer electrodes incorporating polypyrrole and lignin derivatives, coming from brown liquor formed during paper processing, enable charge storage in the quinone functions deriving from lignin. G. Milczarek and O. Inganäs, Science 335 (6075), 1468 (2012).

Biosensors and Bioelectronics

STAFF
Professors: Anthony (Tony) Turner and Fredrik Winquist
Emeritus Professor: Ingemar Lundström
Associate Professor: Edwin Jager
Assistant Professors: Wing Cheung Mak, Ashutosh Tiwari and Valerio Beni
Ph.D. Students: Onur Parlak and Mohsen Golabi.
Research Fellows: Amy Gelmi and Hirak Patra
Visiting Researchers: Dr Raenn Gifford and Dr Douglas Holub
Visiting Scientists: Dr Masoud Mehgard, Dr Janno Torop, Dr Aysu Yarman, Dr Lokman Uzun,
Visiting PhD Students: Daniel Melling, Alina Sekretaryova, Jose Luise Sebastian Avila, Mabel Torrens del Valle, Leila Kashefi, Najmeh Karimian, Jose G. Martinez and Roghayed Iman.
Consultant: Dr Claes Nylander
Managing Editor: Dr Alice Tang
Administrative Staff: Anette Andersson

GENERAL INFORMATION
The division of Biosensors and Bioelectronics expanded rapidly during 2012, averaging around 30 researchers, with the addition of new members including Assistant Professor (Martin) Wing Cheung Mak, post-docs Amy Gelmi and Hirak Patra, Guest Researcher Douglas Holub and PhD. Students Onur Parlak and Mohsen Golabi. Edwin Jager was promoted to Associate Professor. The biosensor laboratory (L202) reached capacity and a comprehensive set of equipment was purchased to support the group’s work in key areas such as electrochemical biosensors, actuators and nano-materials. Our overall mission remains the creation of next generation bioelectronics devices with a focus on distributed diagnostics. More specifically, key strategic targets include fully-integrated biosensing devices, wearable and implantable sensors, non-invasive diagnostics and the creation of new biomaterials.

HIGHLIGHTS
Biosensors for Clinical Analysis:
All-printed Biosensing System
In close collaboration with Acreo AB (Norrköping) and with the invaluable help of Hans Sundgren (Applied Physics), Raeann
Gifford and Tony Turner realised a first demonstrator of an all-printed biosensing system, where not only is the amperometric sensor printed, but all the associated elements such as battery, display and circuitry are printed on a single sheet of PET and then laminated in an appropriate casing. The picture below shows the reality to date, a prototype functioning system. Glucose concentration can be measured in a few seconds and observed via the printed display using this device, powered by a printed battery. Rudimentary silicon circuitry can be seen to the right of the picture, but this could be readily integrated into a tiny, inexpensive silicon chip. This device is being used as a concept demonstrator to develop a range on new products, principally for medical diagnostics.

**Wearable Contact Lens Biosensors with Nanoengineered Architecture Interface. LIST (2012-2013), 350k SEK**

This interdisciplinary project bridges research activity in the Biosensors and Bioelectronics Centre on wearable biosensors for non-invasive ocular diagnostics and work at the Integrative Regenerative Medicine (IGEN) Centre on cornea regenerative medicine for infection-associated corneal transplant rejection. Ocular fluid is an extracellular fluid excreted from the tear gland. With recent advances in proteomic technology, several important biomarkers from ocular fluid have been identified having significant clinical diagnostic value for various diseases. The contact lens is disposable, relatively cheap and serves as a platform to obtain direct intimate contact with ocular fluid, which is an attractive and a promising platform for non-invasive diagnostics. With support from LIST, Masters student Jenny Orban is being supervised by Wing Cheung Mak to develop surface engineering techniques integrating a biorecognition layer onto contact lens surfaces. This exploratory project will serve as a foundation for the future development of wearable biosensors. Our long-term goal is to develop simple, inexpensive and non-invasive contact lens-based wearable biosensors for rapid screening of different potential health risk factors in ocular fluid.

**Enzyme sensors**

**Swedish Institute (2012-2013), 64k SEK**

A key topic for the group is the development of low-cost disposable biosensors for clinical analysis. In close collaboration with Mikhail Vagin (Applied Physics), Valerio Beni and Tony Turner are supervising a visiting student from Lomonosov Moscow State University (Alina Sekretaryova) funded by “The Visby Program – Swedish Institute’s Baltic Sea Region Exchange Program”. Alina is working on two main areas: i) the development of an electrochemical mediated enzyme sensor for the detection of cholesterol and the ii) characterisation of novel mediators for oxidase-based biosensors.

**Cell microencapsulation and monitoring: towards cell therapy**

Delivery of stem cells to target tissues for tissue regeneration is extremely challenging. Stem cell microencapsulation provides a new strategy, which may improve the effectiveness of cell delivery to the target tissue by creating a semi-permeable container separating the encapsulated cells and the environment. In parallel, monitoring of the encapsulated cells inside the microcapsule environment is important to optimise the microcapsule construct design and therapeutic efficacy. We have initiated collaboration with IGEN on integrated stem-cell encapsulation and monitoring for tracking the well-being of the encapsulated stem cells for cell therapy. Master student, Inés Moreno from Cranfield University (UK) is being supervised by Wing Cheung Mak, to develop encapsulation techniques based on hydrogel materials and to perform cell monitoring within microcapsules. The focus is on controlling and monitoring proliferation of stem cells within microcapsules and testing encapsulated Human Umbilical Vein Endothelial Cells (HUVEC) for use as a cardiac patch for heart muscle regeneration.

**Nanobioreactors, stimuli-responsive and intelligent carrier/scaffolds for bioelectronics, drug delivery, imaging and tissue engineering**

Swedish Research (VR) Council (2012-2016) 4m SEK

In addition to our nanobioreactor work described in the previous report, temperature-, pH-, magneto- and photo-switchable nanomaterials are being integrated into high-order diagnostic devices with switchable bioelectronics and modulated biochemical processing. Reversible immunosensors have been designed for the cardiac injury marker, troponin, using both antibodies and molecularly-imprinted polymers. These biomimetic biosensors serve as a model for the design of other affinity sensors for cardiac, genetic and infectious diseases. We are also exploring the use of these smart materials for targeted drug delivery using smart nanocarriers in conjunction with magnetic resonance imaging (MRI) and exploiting their hyperthermic properties for tumor treatment. Stimuli-responsive polymeric unimolecular micelles, formed from pH- and temperature-responsive block copolymers, provide a unique core-shell architecture wherein the hydrophobic core serves as a natural carrier environment for hydrophobic drugs and the hydrophilic shell allows particle stabilisation in aqueous solution. A metallic core can also be introduced into the particle, endowing the particle with optical, magnetic or hyperthermic properties. These novel micelles will contain three key components: (i) a chemotherapeutic agent doxorubicin that will be released from polymeric micelles through a pH-dependent mechanism; (ii) a biological ligand, i.e., specific aptamer that can target tumor cells and subsequently induce receptor-mediated endocytosis for cell uptake; and (iii) a metallic core for ultrasensitive MRI or hyperthermic properties.
**Biosensors for Environmental Analysis:**

*Salmonella typhimurium*

*S. typhimurium* has been identified by the WHO as the most common source of food-borne illness worldwide. Traditionally, microorganisms are detected and quantified by culture and colony count; this is time consuming and requires well-established laboratory facilities. In an effort to reduce analysis time and costs, and to move to on-site analysis, Valerio Beni is working, in collaboration with the Nanobioengineering group at the Institute for Bioengineering of Catalonia (IBEC), Spain, on the development of electrochemical aptamer-based biosensors. As part of this collaboration, Jose Luise Sebastian Avila (PhD student) visited Linköping University for four months. Funded by “The Ministerio de la Ciencia de Espana”, he designed and tested a series of different assay formats using aptamers as recognition/capture elements with enzymatic labels for electrochemical detection.

**Kanamycin A**

Contamination of aqueous environments with pharmaceutical residues has an important impact on the environment and on human/animal health; the presence of antibiotics can promote, for example, multi-drug resistance in pathogens. With the aim of improving water quality, we are developing, in collaboration with the working group “Biological on-site measuring Methods” at the Helmholtz Centre for Environmental Research (UFZ) in Leipzig, Germany, an electrochemical aptasensor for the rapid screening of Kanamycin A in water. This collaboration was generated as part of the COST action TD1003 on Bioinspired Nanotechnologies. The electrochemical biosensor took advantage of the ability of the aptamer, selected at UFZ, to undergo a competition event between the target and an on-surface immobilised probe. Electrochemical monitoring of the recognition event is performed by the use of electrochemical impedance spectroscopy or by the voltammetric monitoring of the presence of a redox centre (Methylene blue) synthetically introduced at one end of the aptamer. The project was supervised by Valerio Beni and carried out by Aristide Ganci, a visiting Master student from Cranfield University (UK) and is continuing by Presty Mathew, a LiU Master student.

**Bioelectronics**

PhD student Mohsen Golabi is investigating a novel concept based on surface interactions to detect and identify different strains of bacteria. We recently expanded this project to include quorum sensing molecules, in collaboration with Dr Elena Vikström and Prof Karl-Eric Magnusson at the division of Medical Microbiology at campus US. A project developing electroactive fibre scaffolds for increased stem cell differentiation, in collaboration with Dr Mehrdad Rafat at Campus US, has gained important momentum from an IGEN grant. Amy Gelmi joined the team in October this year as a post doc to develop these novel fibre-based scaffolds. We have recently fabricated the first fibre mats and are investigating the biocompatibility of the electroactive surfaces. Initial results are promising. Guest researcher, Douglas Holub, started work to investigate synthesis conditions for electroactive materials for the stem cell therapy project, which was made possible by a LiU “U” grant.

**Poly(dl-lactide-co-glycolide) fibre scaffold.**

**Polymer actuators:**

We are currently working on new materials development, micromechanical stimulation, microrobotics and novel actuator designs. We have developed novel polyprrole-based actuator materials to investigate the role of crosslinking in the actuation mechanism. Daniel Melling from Cranfield University, who Edwin Jager externally supervised during his PhD, continues to visit the Biosensor and Bioelectronics Centre as a part of this project. We have a collaboration with the Italian Institute of Technology, Center for Micro-BioRobotics, in Pontedera, Italy, developing all polymer soft actuators and new bioinspired propulsion schemes. As a part of the ongoing collaboration with the Intelligent Polymer Research Institute (IPRI), at University of Wollongong, Australia, Edwin Jager visited IPRI during the summer of 2012 to continue work on microfabricating new soft actuators that work in air. In parallel two MSc students, Nnamdi Felix Nworah and Nirul Masurkar, worked on this project at LiU. We successfully demonstrated new fabrication and interfacing methods and a paper has been submitted. As a part of the COST MP003, Dr. Janno Torop worked on novel PPy hybrid materials. This work resulted in a Carl Trygger Stiftelsen grant and he will join the group as post-doc in 2013. A second STSM was performed by José Martinez, a visiting PhD student from the University of Cartagena, Spain. He stayed in the group for 3 months utilising our specialised laser scanner micrometer for measuring the volume change of PPY as a part of the modeling work on PPy actuation.

**Material/Surface Science:**

**Highly stable surface chemistry for genosensors**

As part of a long-standing collaboration with the Universitat Rovira I Virgili, PhD student Mabel Torrens del Valle came to visit the Centre to investigate the use of micro-contact printing and aryl diazonium salt assembly for the preparation of a highly stable sensing surface for genetic analysis of pathogens. A novel approach based on the catalytic activation of the aryl diazonium salts was developed allowing spontaneous stable grafting of aryl diazonium salt on different substrates such as carbon, Au, Pt and PDOT. The surfaces had high chemical stability and were suitable, following the immobilisation of DNA probes, for electrochemical genosensing. Characterisation of the prepared surfaces is currently ongoing in collaboration with Dr Johan Hurtig (Molecular Physics). The use of the approach for the functionalisation of siliconcarbide and graphene is also under investigation in collaboration with Graphenics.
Automatic synthesis of plastic antibodies

A recent paper in Advanced Functional Materials (Poma et al.) describes an automatic solid-phase photo-reactor developed in collaboration with Cranfield University (UK). At the core of the reactor is an immobilised template, which can be a small molecule, peptide or whole protein. This ensures that surface-confined imprints are formed only on one face of polymer nanoparticles and that the template can be reused for the synthesis of subsequent batches of imprinted polymer. The reactor integrates template-directed synthesis with affinity separation, a combination which ensures the production of monoclonal-type molecularly-imprinted nanoparticles. Batches of 100 mg of particles can be produced in each six-hour cycle with templates including melamine (KD= 7.0x10⁻¹⁰ M), vancomycin (KD= 1.9x10⁻¹⁰ M), a model peptide (5.3x10⁻¹² M) and various proteins (KD= 10⁻¹¹-10⁻⁹ M for trypsin, pepsin, amylase, peroxidase). Affinity measurements were obtained using a SPR sensor (Biacore 3000).

This generic approach to the automated synthesis of polymer nanoparticles provides material of “monoclonal” quality produced in a consistent and reproducible manner, suitable for use as a direct replacement for antibodies in a variety of applications. It offers speed of synthesis and multiple batches of polymer nanoparticles can be produced in 24 h under continuous computer control. Template re-use and in-built affinity separation also ensure consistent, economic and high-quality production.

Another relatively new imprinting approach that is particularly useful for electrochemical sensors uses electropolymerisation of a thin film of the recognition element directly on the sensor surface. The ability to precisely control the thickness of the layer and the fact that it is generated in situ, makes this an attractive alternative. In so far unpublished work, we showed that a troponin sensor could be prepared by electropolymerisation of o-phenylenediamine on a gold electrode in the presence of troponin as a template. Measurements were performed in the presence of 5 mmol l⁻¹ K₃ Fe(CN)₆ and the current generated was inversely proportional to the analyte concentration, since the measurement depends on occlusion of the electrode surface by the template. The resulting molecularly-imprinted troponin biosensor could be used to detect cardiac injury, offering benefits in terms of cost effectiveness, storage stability, sensitivity and selectivity.

TEACHING

The Biosensors and Bioelectronics division has greatly strengthened its role in education during 2012 by designing and giving a series of courses, comprising tutorials, lectures and practical classes. The division runs key courses in the area of biosensors including: Introduction to biosensor technology (TFYA62 – Valerio Beni), dedicated to 2nd year students of the Biomedical Engineering bachelor degree and the advanced Masters course “Biosensors Technology” (TFTB34 – Fredrik Winquist). Edwin Jager presented several lectures for M-cosystem Technology and Nanobiology (TFTB33), Biomedical Materials (TFTB42) and the PhD course Organic Electronics and Tony Turner delivered a number of guest lectures to LiU students. The group has also been engaged at various levels in the design of new courses, mainly at PhD level, that will run from 2013. These include: “Colloids and Interfaces” (Wing Cheung Mak) and Integrated Nanomaterials and Medical Devices (Ashutosh Tiwari). Moreover some of the group have been also involved in design of the course “Experimental Electrochemistry / Electroanalytical Methods”, an effort led by the Biomolecular and Organic Electronics group. Finally the group has been actively involved in the design of CDIO projects (TFTB36 and TBMT41).

BIOGRAPHICAL DETAILS

Valerio Beni

Valerio Beni was born in 1969 in Rome, Italy. He obtained his degree in Electronic Engineering from the University of Rome “La Sapienza” in 1994, where he was awarded a PhD in 1998 for his research on surface-enhanced Raman scattering. He then continued his research at the Paul Drude Institute, Germany, on the catalytic properties of supported platinum nanoparticles. In 2001, he moved to the University of Cambridge, UK, where he worked on the design and development of miniaturized, disposable electrochemical biosensors. In 2004, he joined the Biosensors and Bioelectronics Group at LiU, where he started a programme on the development of immune-based miniaturized sensors for the diagnosis of diseases. In 2008, he moved to the University of Cambridge, UK, as a Senior Research Fellow at the Centre for Bioelectronics. Since 2010, he has been a Professor at LiU, where he is currently the head of the Biosensors and Bioelectronics Group.

The group is involved in the design and development of miniaturized, disposable electrochemical sensors for the diagnosis of diseases. It is currently working on the development of immune-based miniaturized sensors for the diagnosis of diseases.
Biotechnology

STAFF
Professor (head of division): Carl-Fredrik Mandenius
Professor (adjunct): Johan Hyllner
Associate Professor: Gunnar Hörnsten
Research engineer/Lab manager: Robert Gustavsson
Postdoctor: Michael Fritzsche
PhD students: Gunnar Bergström, Inga Gerlach
Research engineer/project: Jonas Cristoffersson
Master students: Cornelia Lukasser, Christopher Darkins, Dan Paulsson, Robin Taponen
Administration: Susanne Andersson/Anna Sundin

SUMMARY
The research and education at the division of biotechnology focus on industrial applications of biotechnology. In essence, industrial biotechnology is the integration of engineering and biology for production purposes. The scientific breakthroughs of the seventies and eighties in molecular genetics, which resulted in the industrial production of recombinant proteins in microbial and animal cell cultures, are now furthered by new products such as stem cells, therapeutic antibodies and gene therapy vectors. A number of bioengineering tools are currently exploited based on genetic, protein, metabolic, physiological and organ engineering in order to improve production capacity of proteins, metabolites, and cells. It is a prime task for the current biotechnology research to integrate and develop these tools in order to achieve and optimize new and better industrial applications. The biotechnology division at IFM is contributing to this by inventing and developing novel analytical means that can provide better insights into the biology of industrial production systems. The cross-disciplinary environment of Linköping University furnishes unique opportunities for this. The combination of sensor technology, mathematical computation methods and production design, supports the use of new approaches that enhance the understanding and allow further optimization of the bio-industrial production systems. The integration of these topics in the curricula of the Engineering Biology program forms an important link between education and research at the division. Our PhD-study program in biotechnology is directly connected to the research of the division and is a part of the research that is highlighted below.

HIGHLIGHTS
Johan Hyllner new adjunct professor

Johan Hyllner, former CEO of the stem cell company Cellartis is now adjunct professor in cell engineering at the division. Cellartis was recently acquired by the French biotech company Cellectis, a world leading company in the stem cell business.

NEW EU PROJECT ON INDUCED PLURIPOTENT STEM CELLS (STEMBANCC)
The division has together with 40 partners received a five year IMI project – STEMbancc - on induced pluripotent stem cells.

The aim of the project is to generate and characterise 1 500 high quality human induced pluripotent stem (iPS) cell lines that can be used by researchers to study a range of diseases, including diabetes and dementia, and test for drug efficacy and safety. The cell lines will help to improve and speed up the drug development process, and ensure that patients benefit from more effective and safer drugs. Mandenius is the leader of the in vitro assay development in the project.

NEW PROJECT ON LAB ON A CHIP FOR TOXICITY TESTING
Together with the group of Dr Nate Robinson at IFM we study new designs of Lab on a Chip for toxicity testing. The project is supported by the Swedish Research Council program for reducing animal testing.

SOFT SENSORS FOR BIOPROCESS MONITORING AND CONTROL
Soft sensors are robust on-line sensors supported by mathematical models derived from the systems under study. In particular, they are useful for bioprocess monitoring due to the complexity of the biological mechanisms of the producing cells. We have used soft sensors to monitor physiological signals from typical industrial cultures by combining sensors for biomass, effluent gases and key metabolites with basic mass balances and kinetic (Gustavsson and Mandenius, Bioprocess Biosystems Engineering, 2012). Also, a conference talk was given by Robert Gustavsson at the 15th European Congress of Biotechnology in Istanbul.

BIOMECHATRONIC DESIGN IN BIOTECHNOLOGY
In collaboration with IEI at LiU we have continued studies on the industrial development and design process of complex biotechnology instruments and devices. During 2012 we have followed up this topic with several new research articles and conference talk (see publication list).
Conceptual design solutions from a biomechatronic approach

VIRTUAL BIOREACTOR TRAINING
In collaboration with the University of Applied Science in Bremen, and with support from PUG at the technical faculty, we have continued to develop new virtual tools. One of these is a virtual bioreactor that mimics the operator environment in a biotech production plant. It allows the engineering students to apply monitoring and control methods in a hands-on fashion. The goal is to strengthen the link between engineering theory and practice with the aim to make the students better prepared for professional life.

A virtual bioreactor used for training master students in engineering biology

EDUCATION
The division has during 2012 delivered three advanced level courses in the Engineering Biology/Chemical Biology programs (Industrial Biotechnology, 6 hp; Bioprocess design, 6 hp; and Bioprocess manufacturing, 6 hp) and examined several diploma work theses in biotechnology.

Molecular Physics

STAFF
Professors: Bo Liedberg (on leave), May Griffith.
Associate professors: Thomas Ederth (acting head of division), Karin Enander.
Assistant professors: Daniel Aili, Johan Hurtig.
Post-docs: Li Buay Koh, Jaywant Phopase, Luigi Petrone, Staffan Dånmark.
Visiting scientists: Ramunas Valiokas, Alexander Onipko, Sushanth Gudlur.
Administrative and technical staff: Therese Lindkvist, Anna Maria Uhlin, Bo Thunér.
Guest professor: Atul Parikh, UC-Davis

2. SUMMARY
The division of Molecular Physics conducts fundamental and applied research in three closely related fields of biologically inspired surface and nanoscience: Biosensing and biochip technology; molecular/polymer thin film physics and spectroscopy; and nanoscale physics/chemistry. The fundamental part of the biosensing and biochip research is devoted to the design and synthesis of surface active compounds and new biorecognition molecules. Polypeptide as well as carbohydrate recognition molecules are synthesized and evaluated using the above mentioned transducer platforms. We are also working with de novo synthesized helix-loop-helix polypeptides and minimized sequence peptides for microarrays. A significant portion of the research utilizes solution self-assembly techniques to produce novel surface architectures and materials. A new type of oligomeric monolayers forms the base for our investigations, and through a fruitful combination of surface vibrational spectroscopy and quantum chemical ab initio calculations we have improved the understanding of the mechanisms that influence the phase behaviour and orientation in such layers.
Several projects utilize nanoparticle plasmonics for sensing applications. We are particularly interested in using gold and silver particles for studies of metal-enhanced optical phenomena such as metal enhanced extinction (MEE) or metal-enhanced fluorescence (MEF), or using localized surface plasmon resonance (SPR) for improved imaging. Some of these projects are carried out with the School of Materials Science and Engineering, Nanyang Technological University, Singapore. The plasmonic research also relates also to our activities on helix-loop-helix polypeptides for controlled aggregation of gold nanoparticles (NPs) into functional entities.
Our long-standing research on antifouling surfaces has somewhat shifted focus from biomedical to marine biofouling applications over the last few years, and is now conducted primarily through our involvement in the Marie Curie Initial Training Network SEACOAT. The network involves research in three complementary, interdisciplinary themes: surface engineering, surface analytics and bioadhesion. An important part of our research in marine biofouling is the development of real-time methods for monitoring of surface interactions of...
marine organisms. For this purpose, a recently acquired laser-TIRF microscope with an integrated imaging SPR facility will be of great importance.

The Molecular Physics division is deeply involved in the initiative on Regenerative Medicine headed by Prof May Griffith, and which is now in its third year. The laboratories for polymer science and peptide chemistry at the division serve other partners in the project with new materials and molecules, and also provide advanced tools for the characterization of the developed materials and implants, thus contributing to a concerted effort to make translational technologies (bench-top to bed-side) a reality.

Staff at the division are also involved in undergraduate teaching, giving advanced courses on surface and supramolecular chemistry, spectroscopy and biomedical materials.

Daniel Aili was recruited as a LiU-Forskarassistent in 2011 and has during 2012 received extensive funding from both the Swedish Foundation for Strategic Research (Ingvar Carlsson Award) and the Swedish Research Council (VR) to pursue research on responsive hybrid materials, leading to a considerable expansion of the division over the last year. Aili was also awarded the AkzoNobel Nordic Prize in Surface and Colloid chemistry.

3. HIGHLIGHTS
Chelation assisted photoimmobilization – a novel route to covalent, oriented protein immobilization
Karin Enander, Bo Liedberg, PhD student: Emma Ericsson. A novel two-step method for homogenous orientation and covalent attachment of His-tagged proteins to sensor surfaces has been developed, where a chelating agent (nitrilotriacetic acid, NTA) captures the protein in an oriented fashion followed by covalent tethering by the reaction with a photolabile group (benzophenone, BP). The strategy was demonstrated on gold sensor surfaces with mixed self-assembled monolayers of NTA- and BP-presenting alkanethiols. Although homogeneous ligand orientation is less crucial for analyte accessibility in the case of multivalent ligands, this strategy may prove very useful for monovalent ligand-analyte interactions, offering a well-defined mode of immobilization suitable for microchip photopatterning applications.

Detailed molecular characterization of thrombin-par4 interactions
Karin Enander, PhD student: Robert Selegård. In a recently formed collaboration with Prof Tomas Lindahl and Dr Sofia Ramström (Laboratory for Clinical Chemistry, Department of Clinical and Experimental Medicine, LiU) we use surface plasmon resonance-based analysis to characterize low-affinity interactions between thrombin and polypeptides corresponding to the extracellular loops of the human PAR4 receptor expressed on platelets. Our ambition is to map sites in both thrombin and the receptor that contribute to the interaction, which is crucial for platelet activation during blood coagulation.

Interfacial charge and swelling of layered polyelectrolyte hydrogel gradients
Thomas Ederth, PhD student: Feng-I Tai. Hydrogel patterns and gradients are of immediate interest for biochip and protein array technology. In sandwiched thickness gradients of anionic and cationic polymers, charge neutral regions are very resistant to non-specific protein adsorption. We have prepared two-component hydrogels (Figure 1) with a charged uniform bottom layer, an oppositely charged thickness gradient is grafted. The location of the charge neutral region along the gradient depends on the pH, and direct force measurements using a charged colloidal probe is used to study the complex swelling behaviour of the hydrogels and monitor the shift of this minimum as the pH is changed.

Figure 1. Top: schematic of a two-component hydrogel gradient. Below: AFM force curves obtained using a negatively charged probe on a P(AEMA-CEA) gradient, showing re-location of the charge-neutral region.

Lipid membrane architectures
Johan Hurtig. Funds from the Magn. Bergwall and Carl Trygger Foundations have permitted acquisition of a fluorescence microscope with an ultrasensitive camera detector. This is used in projects related to control of directional growth of intercellular nanotubes through micropatterned substrates as well as nanosurgical extraction of cell material. The investigation of intercellular nanotubes is based on an interdisciplinary approach between microfluidic sample handling, nanomarked substrates and sensitive detection technologies to probe a new eukaryotic cell-cell communication strategy.

Mechanisms for lysosomotropic destabilization of membranes
Thomas Ederth, PhD student: Timmy Fyrner. Lysosomes are vesicular organelles found in virtually all eukaryotic cells and are involved in macromolecule turnover and thus contain numerous hydrolytic enzymes, digesting unwanted material in the cell. Lysosomes are also involved in apoptosis; the lysosomal membrane is permeabilized in response to cell death stimuli, although the mechanisms behind this are poorly understood. In collaboration with Karin Öllinger (Faculty of Health Sciences, LiU), and Atul Parikh (UC Davis) we investigate mechanisms for lysosomal membrane destabilization by natural and synthetic lysosomotropic detergents.

Local refractive index sensing based on metal nanostructures
Bo Liedberg, Daniel Aili, PhD students: Erik Martinsson. We develop optical biosensors based on detection of small local refractive index changes in the vicinity of metal nanostructures. In cooperation with a group at the School of Materials Science and Engineering, Nanyang Technological University, Singapore we have explored the bulk and surface refractive index sensitivity of core-shell Ag@Au nanoparticles, finding that these are much more sensitive to local refractive index changes than both conventional surface plasmon resonance as well as spherical gold nanoparticles (Figure 2). We aim to integrate these nanostructures as sensing elements in optical biosensors in order to monitor biomolecular reactions occurring in the proximity of the nanostructures.
Peptide-polymer hybrid materials
Daniel Aili, Post-doc: Staffan Dånmark, PhD student: Christopher Aronsson. We develop peptide- and polymer hybrids for self-assembly of hydrogels with well-defined and tunable properties for biomedical applications. The peptides are designed to fold into coiled-coil heterodimers with high structural integrity, low KD for dimerization, and controllable/tunable assembly- and oligomerization-properties. The peptides are modified to promote polypeptide fiber-formation but can also be covalently attached to polymer scaffolds based on hyaluronic acid and polyethylene glycol. Polymer scaffolds are currently being modified for conjugation with the peptides.

Self-assembly of anisotropic nanostructures
Daniel Aili, Karin Enander, PhD student: Camilla Sandén. The aim of this project is to develop well-defined and biocompatible nanoscale components for modular self-assembly of anisotropic hybrid materials using reconstituted high-density lipoprotein (rHDL) as a supramolecular template. The rHDL is functionalized to specifically associate with gold nanoparticles and to form well-defined and discrete nanostructures with interesting and useful optical properties. The synthesis of rHDL has been optimized and several strategies for functionalization and assembly of the nanostructures have been evaluated.

Collagen-based scaffolds and hydrogels
May Griffith, PhD student: Abeni Wickham. A large focus is on development of different strategies for collagen scaffold formation. We are now able to make the collagen and cellulose as a hydrogel (90% water), collagen electrosprun fibers, and highly dense collagen meshes (5% water). The latter material is very similar to the Apligraf® used for wound treatment and has now become the material emphasis for the collaboration with Linköping University Hospital’s burn unit. In collaboration with Prof Juan Scaiano and Dr. Emilio Alarcon of Ottawa University, silver nanoparticle/collagen composites have been developed demonstrating excellent antibacterial activity. The joint work with groups supplying electroactive polymers still continues and motions are underway to move those materials into proper animal models.

Cell response regulation on collagen surfaces with patterned peptides
May Griffith, Bo Liedberg, PostDocs: Li Buay Koh, Jaywant Phopase. The aim of this research is to stimulate an enhanced growth of cells for clinical applications as biomimetic corneal substitutes. Micropatterns of laminin-derived cell-adhesive peptides (YIGSR-NH2 and IKVAV) with varying dimensions were grafted onto a collagen layer and subsequently seeded with various cell types to investigate for the cell responses. Our results showed the attachment, alignment and proliferation of human corneal epithelial cells on the patterned surfaces with IKVAV as shown in Fig. 1. Current studies which involve other cell types (e.g. neuroblastoma and stromal cells) and investigation on the cells proliferation rate on these modified surfaces is ongoing.

Regenerative Medicine

Linköping Integrative Regenerative Medicine Centre (IGEN), funded by LiU and the County of Östergötland, enables multidisciplinary teams to work together to develop bold innovative treatment methods that will restore function to damaged or diseased organs and tissue. The activities within regenerative medicine at IFM include design and preparation of new biomaterials and bioactive molecules, and provision of advanced tools for the characterization of the developed materials and implants.
Molecular Surface Physics and Nano Science

Development of Template-Assisted Supramolecular Assembled Collagen-Mimetic Hydrogels

May Griffith, Bo Liedberg, Jaywant Phopase.

Our objective is to develop designer scaffolds using polymeric multiarm templates conjugated with collagen-mimetic peptides (CMPs) which can self-assemble into collagen-like triple helical networks. Collagen forms the basic scaffolding of virtually every organ, but is susceptible to enzymatic degradation. This can be circumvented by CMPs with the desired properties of collagen but whose stability can be controlled. A CMP conjugated with 8-arm PEG maleimide template forms a self-supporting transparent hydrogel suitable for corneal implant. The hydrogel supported the growth and proliferation of human corneal epithelial cells and has shown significantly higher enzymatic stability compared with EDC/NHS cross-linked human recombinant collagen hydrogels, currently in phase-2 human clinical trials for the corneal regeneration.

Figure 5. a) Attachment of the human corneal epithelial cells on the grafted patterns with IKVAV at 6 hrs and b) cells proliferation along the peptide patterns at 48 hrs with live dead staining of the cells.

Figure 6. Assembly of CMPs into scaffolds.

STAFF

Professor: Kajsa Uvdal
Junior Researcher: Xuanjun Zang, Caroline Skoglund
Postdoc: Zhangjun Hu
PhD students: Cecilia Vahlberg, Maria Ahrén, Linnéa Selegård, Linnéa Axelsson, Natalia Abrikossova, Emanuel Larsson
Diploma students: Emanuel Larsson
Technical staff: Bo Thunér
Administrative staff: Anna Maria Uhlin, Therese Lindkvist

GENERAL

The division of Molecular Surface Physics and Nano Science is a division at Applied Physics IFM, active in the field of Nanomaterial and Molecular thin film physics and spectroscopy. Our main focus is on surface modification for sensing/biorecognition and nanoparticles for biomedical imaging. Biospecific binding phenomena at solid surfaces are investigated. Design and characterization of new and improved nanoparticles for imaging are performed. Equipment used are X-ray Photoelectron Spectroscopy (XPS), Photoemission electron Microscopy (PEEM) Near Edge X-ray Absorption Fine Structure (NEXAFS) Spectroscopy, Infrared Absorption Spectroscopy (IRAS), Dynamic Light Scattering (DLS), Transmission Electron Microscopy (TEM), computed tomography (CT) and Magnetic Resonance Imaging (MRI). Super small particles i.e. particles with very small volume, with unique physical and chemical properties, have a high potential in biomedical imaging and future biosensing applications. We are designing biocompatible nanoparticles based on rare earth metal oxides. These are very promising as positive contrast agent (Patents) in MRI and CT. Powerful equipment available at IFM, in house experience of life science technology and molecular physics as well as close collaboration with CMIV (Center for Medical Image Science and Visualization) facilitate progress in the field of novel nanomaterial design for bio medical imaging. Research based on the use of synchrotron radiation is of main importance for our research group and is conducted at MAX II Swedish national laboratory in Lund and at Elettra Trieste Italy. MAX II is a third generation electron storage ring for synchrotron radiation. The techniques used are high resolution X-ray Photoelectron Spectroscopy (XPS) and Near Edge X-ray Absorption Fine Structure (NEXAFS spectroscopy) This year we have expanded our activity to computed tomography (CT) at the synchrotron facility at Elettra Trieste in Italy.

TEACHING

A yearly course in Surface Science (TFTB35) which is an Undergraduate profile courses, 4th year for students on the programmes Chemical Biology and Engineering Biology, is conducted in our research laboratories. The students obtain hands on experience in using powerful techniques and equipment in
applied physics

surface science. The projects and molecular systems chosen are closely related to issues in biomolecular surface modification research. A new course Material for biomedical engineering –from nano to macro level (TFYA63) was developed and given for students enrolled in the Biomedical Engineering program. The course deals with biomaterials and their interaction with human cells and tissues and is composed of lectures and seminars as well as extensive laboratory exercises.

THE PHD PROGRAMME
The PhD students within the division of Molecular Surface Physics and Nano Science are enrolled in the graduate school Forum Scientium.

HIGHLIGHTS

Nanoparticles for biomedical imaging In this project we are designing and characterizing rare earth nanoparticles to optimize the contrast in magnetic resonance imaging (MRI). This project includes material design and synthesis, characterization, surface modification, biofunctionalization and signal optimization followed by tagging for targeting purposes.

The synthesis of the material is done in close collaboration with Inorganic Chemistry and bioorganic chemistry, IFM. The MR signal optimization is done in cooperation with the Center for Medical Image Science and Visualization (CMIV) at the medical faculty and University Hospital. We have shown that the relaxation properties of this contrast agent have an enhancing capability with respect of MRI signal, compared to the commercially available ion based Gd-DTPA contrast agent. With this new contrast agent the aim is to obtain higher resolution, tissue specific images and cell- and molecular imaging. Knowledge obtained with in the project will contribute to the understanding of drug delivery targeting. Our goal is to improve the contrast to enable high resolution imaging for e.g. early diagnosis of neurodegenerative diseases and cancer. This is a true interdisciplinary project, combining Physics, Chemistry, Biology and Medicine.

Multifunctional Nanoprobes for Tumor Diagnosis One fundamental part of the biomedical imaging research is devoted to the design and synthesis of new recognition nanoprobes and to their capability for signal enhancement. A new interdisciplinary project involving Applied Physics, Organic chemistry, Pharmacology, CMIV and Clinical and Experimental Medicine to develop nanoprobes for biomedical imaging and tumor targeting. Our vision is to design calcium-receptor targeted nanoprobes with luminescence and magnetic properties, with the capability to specifically image.

Supramolecular approach to nanoscale metal-containing gels, fibers, belts, and rods. The ligand-structure effect and mechanism of 1D growth of nanofibers have been studied. Cu-Li acts as “super-gelators” representing one of the rare examples of metallogelators with very good selectivity to Cu(II) over other metal ions. These dynamic gels and nanofibers exhibit solvent mediated shape transformation by stimulation of ultrasound. The shape control and the study of the structure effect at the molecular level in this work will certainly expand the synthesis of 1D metal-containing nanostructure in the development of new functional materials.

Figure 1. A). Transmission electron microscope images of one Gd₂O₃ based nanoparticle, B) Schematic illustration of one surface modified nanoparticle C) Image of X. laevis fibroblasts exposed to Nanoparticles D). MR image of the human brain.

Figure 2. A). Transmission electron microscope images of one Gd₂O₃ based nanoparticle B) Schematic illustration of surface modification including specific tag both for plane surface and nanoparticle systems
Figure 3. Left: molecular structure of ligand H2L1; right: TEM and SEM images of L-Cu nanofibers and photoimage of the ligand after addition of different metal ions.

Nanoparticles and human living cells Studies investigating the interaction between nanoparticles and human living cells and tissues are of great importance in the further development for e.g. nanoparticles for biomedical imaging. We have performed studies to clarify the effects of Gd2O3 nanoparticles on neutrophil granulocytes and we show that functionalization of the particle surface is essential in order to maintain a healthy cell response upon neutrophil exposure to nanoparticles.

Figure 4. Left; fluorescent Gd/Zn nanoparticles phagocytosed by neutrophil granulocytes. Right; Schematic illustration of experimental setup evaluating the effect of nanoparticle exposure on the production of reactive oxygen species.

RESEARCH COLLABORATIONS M. Engström and A. Persson Center for Medical Image Science and Visualization (CMIV) S. Svensson, Pharmacology HU. M Griffith, Nanomedicine, Health University Linköping, Prof. P. Norman, Computational Physics, Linköping University Prof, R. Yakimova, Prof. A. Lloyd Spetz, Applied Physics Liu Åbo Finland, T Bengtsson Örebro, LIU Cancer network, IGEN centre which is strategy area of regenerative medicine University M Lindgren NTU Trondheim Norway, MaxLab Swedish National Laboratory in Lund, J Tromba Elettra Trieste Italy, C Dullin Germany S. S. Venkatraman NTU Singapore Industry partners Vironova,AB SPAGO Imaging AB Lund.

THE CENTRE IN NANO SCIENCE AND TECHNOLOGY (CeNano) is an organization within the Technical Faculty of Linköping University. The mission of CeNano is to strengthen and support the competence within nano science and nano technology of the faculty. This is made by gathering researchers with nano activities in the centre and by acting for increased collaborations and common projects in the nano realm. CeNano also acts for development and coordination of the graduate and under graduate education in this scientific area. K. Uvdal is the director of CeNano.

Applied Sensor Science

STAFF
Professor: Anita Lloyd Spetz
Scientists: Dr Mike Andersson, Dr Robert Bjorklund, Dr Jens Eriksson, Dr Donatella Puglisi
Administrative staff: Theresse Dannetun
Graduate students: Zhafira Darmastuti, Christian Bur, Hossein Fashandi
Research engineers: Peter Möller

RESEARCH ACTIVITY
Division of Applied Sensor Science participates in several research organizations within IFM: The Vinn Excellence Center FunMat (Lloyd Spetz acting Deputy Director), Advanced Functional Materials, AFM, and in projects within Applied Physics, Material Science and Chemistry Division. The COST Network, EiNetAir TD1105, with partners from 25 countries was launched in May 2012. The network acts in the field of New Sensing Technologies for Air-Pollution Control and Environmental Sustainability. Lloyd Spetz was appointed Deputy Chair of the network.

Lloyd Spetz is acting FiDiPro, Finnish Distinguished Professor at Oulu University at 50%, 2011-2014. The research project concerns development of a portable nanoparticle detector for detection of number, size, shape and content of particles.

NEW GENERATION SiC-FET GAS SENSORS
A new generation of SiC-FETs developed by the spin-off company SenSiC AB in collaboration with Applied Sensor Science and FunMat, shows largely improved sensor characteristics in terms of selectivity, sensitivity and long-term stability. It is also possible to fine-tune the operation parameters when using the sensors for alarm purposes simply by adjusting an offset voltage, as demonstrated for ammonia in the top right figure. The new FET sensor generation also allows for better control of sensor operation parameters such as operation temperature and automatic zero point calibration.

Upper panel: flue gas emissions of CO (red) and ammonia slip (blue). Lower panel: The corresponding sensor signal (gate electrode, iridium) set to an alarm level of 15-20 ppm ammonia.
GRAPhENE SENSORS
Mono- and bilayer graphene, epitaxially grown on SiC in the group of Prof Rositza Yakimova, Material Science Div was characterized for gas sensing and shows ultra-low detection limit, less than 10 ppb of NO₂. It was shown that upon exposure to electron acceptors (oxygen, water vapour, NO₂) or donators (NH₃), the relative Fermi level in single layer graphene suffers a greater change than that in bilayer graphene. (R. Pearce, J. Eriksson, T. Jakimov, L. Hultman, A. Lloyd Spetz and R. Yakimova, ACS nano, accepted). The graphene sensor research is supported within FunMat and AFM - Strategic Faculty Grant in Advanced Functional Materials. A patent was filed regarding a smart sensor device based on graphene/ SiC. Also MAX based mono- or few layer materials like MXene (TiC) are investigated according to gas sensing properties.

Operation modes like cycling of the operation temperature or applied bias are designed and together with smart data evaluation the information from SiC sensors is largely improved. Interesting results were obtained like simultaneous quantification of both NO and NO₂ in a (varying) mixture of synthetic exhaust. Christian Bur has a position as PhD student in this project at both Saarland and Linköping Universities within the research school DocMASE.

FUNMAT
The VINNOVA VINN Excellence center FunMat, is also presented elsewhere. We run projects with industrial partners (Alstom Sweden AB, SenSiC AB, Volvo Technology, Ford Motor Company) focused on MAX materials (conducting ceramics) for ohmic contacts to SiC, new sensing layers for SO₂, H₂S, NO/ NO₂ and O₂ and a soot sensor for diesel exhausts.

METHANOL SENSOR
In a joint project with Chemistry Division, Profs. Per-Olov Käll and Lars Ojamäe, the synthesis of methanol, with potential as a biofuel, from CO₂ and H₂ is studied. Methanol is toxic and therefore we develop a sensor as an alarm for this gas and for process control.

SIC BASED AMMONIA SENSORS FOR CONTROL OF SNCR
This project was initially supported by VärmeForsk and involves the industrial partners, Tekniska Verken, SenSiC AB, Vattenfall and Alstom Power Sweden AB. It concerns development of a SiC based ammonia sensor system to control SNCR (selective non catalytic reduction), i.e. injection of ammonia (or urea) in hot flue gases in order to convert nitrogen oxide gases to nitrogen and water. It continued partly on faculty support during 2012. Now an ammonia sensor, also intended for stationary engines, is commercially available through SenSiC AB.
Surface Physics and Chemistry

STAFF
Professors: Mats Fahlman (Head of Division), Koungh-An Chao (Emeritus), William R. Salaneck (Emeritus)
Associate professors: Nathaniel Robinson
Research engineers: Slawomir Braun, Xianjie Liu
Postdocs: Shengwei Shi, Zhengyi Sun
PhD students: Qinye Bao, Katarina Bengtsson, Per Erlandsson, Sara Nilsson, Parisa Sehati
Administrative staff: Kerstin Vestin

SUMMARY
The division consists of two research groups: Organic Physics (Fahlman, Bao, Braun, Liu, Sehati, Shi, Sun) and Transport and Separations (Robinson, Bengtsson, Erlandsson, Nilsson). The Organic Physics research consists of fundamental study and model development of weakly-interacting organic and organic-metal interfaces; interface engineering in organic electronics i.e. development of techniques for improving charge injection, excitation dissipation and stability of interfaces in organic electronic devices; transparent conducting electrodes (graphene, inorganic oxides) and their interaction with organic electronic materials; intrinsically conducting polymers such as PEDOT and PANi: the effect of synthesis and choice of (poly)anion on conductivity, biocompatibility and general surface properties.

The Organic Physics group also does research focused on the study and design of hybrid organic spintronic interfaces (spin-particles) with the aim to understand and improve devices such as hybrid spin-valves; and the development and study of thin film organic-based semi-conducting magnets such as V(TCNE)x, x~2, with an emphasis on achieving work function tailoring. (MPIP, IMEC in MOLESOL).

Continued development of the Integer Charge Transfer Model focused on molecular order effects and energy gradients over multilayer systems was carried out in collaboration with Geert Brocks and Michel de Jong of the University of Twente (MINOTOR).

Ultraviolet photoelectron spectroscopy, optical absorption, photoluminescence, and charge carrier mobility versus temperature data was used to determine the contributions from the polaron binding energy and energetic disorder on the hole-transit properties of poly(3-hexylthiophene).

By combining XPS, UPS and NEXAFS, we studied the interface interaction and energy level alignment between dye molecules (EPFL, IMEC in MOLESOL) and TiO2, shedding light on the importance of surface defects states in the TiO2 nanocrystals.

By combining XPS, UPS and NEXAFS, we studied the chemical interactions, energy level alignment and degradation effects of materials and interfaces constituting tandem solar cells (Geneslink, BASF, Chalmers, AGFA-Gaevert in SUNFLOWER).

Repair and renovation was carried out on the Scienta and MOSES photoelectron spectrometer systems.

Emeritus professors
- Prof. Salaneck attended the March meeting (solid state physics) of The American Physical Society, Boston, MA, USA; the "Fest-shrift" for Prof.-Dr. Klaus Müllen, Shanghai, China; the 50th Anniversary of the foundation of the Laboratory for Research on Structure of Matter (LRSM) at the University of Pennsylvania, Philadelphia, PA, USA; the ICSM-2012 (International Conference on Synthetic Metals), in Atlanta, GA, USA, where he was Chairman for "Surfaces and Interfaces".
- Prof. Salaneck is a member of the Board of Directors for an SME and a Vinnova project.

Organic Physics group
- By combining XPS, UPS and NEXAFS, we studied the interface interaction and energy level alignment between dye molecules (EPFL, IMEC in MOLESOL) and TiO2, shedding light on the importance of surface defects states in the TiO2 nanocrystals.
- By combining XPS, UPS and NEXAFS, we carried out engineering characterization of graphene and NCD surfaces, with an emphasis on achieving work function tailoring. (MPIP, IMEC in MOLESOL).
- By combining XPS, UPS and NEXAFS, we studied the chemical interactions, energy level alignment and degradation effects of materials and interfaces constituting tandem solar cells (Geneslink, BASF, Chalmers, AGFA-Gaevert in SUNFLOWER).

Transport and separations group
- The Transport and Separations Group has initiated several projects in the area of microfluidic devices.
- Our LIST project in collaboration with the Imaging and Ubiquitous Chemical Sensing Lab at IFM and the Cell Biology group at IKE has resulted in microfluidic devices for use in measuring fucose in urine.
- We have begun making and testing microbioreactors with...
our partners in the Biotechnology group at IFM. These devices are intended to help reduce the need for animal testing during chemical toxicity and pharmaceutical evaluations.

We have also initiated a project with the Clinical Chemistry Group at IKE to design microfluidic systems for studying and analyzing the activation of platelets in blood by shear stress.

- One of the most exciting areas of development is the use of 3D printing (fabbing) to produce microfluidic devices. We use a 3D printer capable of extruding soft materials like polymers, allowing us to take advantage of our previously-developed technologies such as the polymer electroosmotic pump and making our research rather unique in the world.

**COOPERATING PARTNERS AND VISITING SCIENTISTS**
The different international universities, institutes and companies with which funding were shared in projects during 2012 are listed below:

**EU-FP7 MINOTOR:** University of Mons, University of Twente, Interuniversitair Micro-Electronica, University Bordeaux, Bologna University, Universidad Autonoma de Madrid, BASF, Forschungszentrum Karlsruhe and Georgia Institute of Technology.

**EU-FP7 MOLESOL:** IMEC (Belgium), J. Heyrovsky Institute of Physical Chemistry of The Academy of Sciences of the Czech Republic, Ecole Polytechnique Federale de Lausanne, Max-Planck Institute for Polymer Research, SolarPrint Ltd, Greatcell Solar.

**EU-FP7 HINTS:** ISMN-CNR, Martin Luther University Halle-Wittenberg, NanoGUNE, Trinity College Dublin, Jožef Stefan Institute, Queen Mary University of London, University of Kaiserslautern, Universitat de València, Dr. Eberl MBE-Komponenten GmbH, M-Solv, THALES Group, CNRS PALAISEAU.

**EU-FP7 SUNFLOWER:** CSEM, BASF AG, DuPont Teijin Films, AMCOR Flexibles, AGFA-Gaerert NV, Fluxim AG, Konarka Technologies, SAES Getters, CNR – ISMN, Fachhochschule NordwestSchweiz, Chalmers, FhG IVV & ISC, Universitat Jaume I de Castellon, GenesInk, CNRS, University of Glasgow.

We also received a visit from Martin Kronstein from the Vienna University of Technology.

There are many other partners in co-publishing activities outside of the co-financed projects as well.

**INTERACTION WITH SOCIETY**
Commercialization efforts are underway for both the LEC and microfluidic research via Lunavation AB.

We assist the industrial partners in their commercialization efforts in the various EU FP7 projects.
SCIENTIFIC BRANCH OF

Biology

STAFF

Professors: Mats Amundin (adjunct professor), Per Jensen, Jan Landin (emeritus), Matthias Laska, Per Milberg
Associate professors/Senior lecturers: Agneta Johansson (Director of studies), Ricky Ansell (adjunct), Jordi Altimiras, Kristina Blomqvist, Johan Edqvist, Karl-Olof Bergman, Jenny Hagenblad, Anders Hargeby, Ronny Lock, Karin Tonderski, Jennie Westander (adjunct), Thomas Östholm
Assistant professors: Heidi Paltto, Hanne Lovlie, Lina Roth, Dominic Wright, Lars Westerberg, Matti Leino
Junior lecturers: Kjell Carlsson, Eva Mattson, Orjan Lönnvik, Åsa Rybo Landelius
Other teaching staff (part time): Johan Bergstedt
Post doc: Rie Henriksen, Vivian Goerlich, Isa Lindgren, Niklas Jansson, Daniel Nätt (50% IKE), Hugo Oliveira, Ann-Charlotte Svensson-Jolin
PhD-students: Beatrix Agnvall, Johan Beltéky, Hristina Bodin, Maria Ericsson, Amir Fallahshahroudi, Nils Forsberg (NTU), Pernilla Foyer (FHS), Magnus Elfwing, Karin Johansson, Martin Johansson, Anna-Carin Karlsson, Håkan Lättnan, Pia Lövstedt, Helena Olsson, Monika Malmbecker Edstam, Josefín Starkhammar (LU), Daniel Wennergren, Josefina Zidar, Anders Wirén, Hanna Österman
Administrative/Technical staff: Ingevald Abrahamsson (Engineer), Lejla Bektic (Animal Technician), Tove Berg (Technician), Maria Lundström (Lab Technician), Jessica Lövdahl (Administrator), Mia Persson (Lab Technician), Andrey Hoglund (Lab Technician), Eva-Maria Stigsdott (Administrator), Anna Sundin (Administrator)

Biology covers all aspects of life science, from subcellular molecular processes, via organisms to whole ecosystems. Basic scientific challenges in the area concern the way in which genetic instructions influence the development of organisms, which interact and constitute a complex biological system. This is knowledge, which is strongly requested from society. It influences a wide range of societal issues from the use of gene technology for altering and affecting the function of various organisms, to questions of animal welfare in modern farming and the management of species and ecosystems for biological conservation purposes.

IFM Biology has about 60 persons employed in total, of which about 20 are PhD-students. To organize and lead the activities, the branch has a steering committee, which includes the head of division, two assistant heads of division, and the director of studies. This group meets every week and is responsible for matters concerning budget, teaching, research, PhD-education and organization.

Within IFM Biology, the research is organised in research groups, which are ad hoc associations of people working on a common scientific theme. The groups are dynamic, and can change their composition as deemed suitable by the involved people. In the following pages, the research groups active during this year present their activities.

The PhD-education is carried out within four different subjects: Ecology, Zoology, Ethology and Molecular Genetics. Within Ecology, emphasis is on community and population ecology, including conservation biology, vegetation and wetland ecology. Here, methodology and temporal trends have been studied in areas such as phenotypic plasticity and seed dormancy. In Molecular genetics, research training is focusing on plant molecular biology. In Zoology, research is mainly focused on developmental aspects of cardiovascular control systems and comparative olfaction research, and in Ethology, focus is on domestication effects on behaviour in chickens. The staff is also heavily involved in undergraduate teaching in all subjects covering the biological education programs.

IFM Biology has had an excellent success rate in external funding over the last couple of years, and important grants were also obtained 2012. For example, researchers from the branch were awarded project grants from both VR and Formas. Professor Per Jensen, professor Per Milberg, and Senior lecturer Jordi Altimiras hold contract supports from the University, and Professor Per Jensen was awarded an ERC Advanced Researcher Grant.

Research facilities include the research chicken house ("Wood-Gush") and the hatchery ("Krujit"), along with state-of-the-art molecular lab facilities.

Staff from IFM Biology was instrumental in planning and organizing a popular science day, with parallel sessions containing lectures in biology, chemistry, physics and mathematics. The lectures attracted in total about 1000 attendants, mostly school teachers and high school students.

IFM Biology has a wide-ranging collaboration with groups and labs in different places of Sweden and abroad. For example, cooperation in both teaching and research is maintained with groups in Bolivia, The Netherlands and Great Britain. Furthermore, the cooperation with Kolmården Zoo has continued and produces both research results and teaching collaboration.

Chickens are important model animals in the Division of Zoology.
Their behaviour, genomics and physiology are studied in a number of research projects.
The AVIAN Group includes research on behaviour (Per Jensen) and personality (Hanne Løvlie), physiology (Jordi Altimiras) and genetics (Dominic Wright).

Although not restricted to it, most of the group’s research focuses on the ancestral Red Junglefowl and modern chicken breeds selected for farming purposes such as egg productivity or meat yield with the goals of understanding the genetic basis of animal domestication and its functional mechanisms.

As part of the Centre of Excellence in Animal Welfare Science our research is also dedicated to the improvement of animal welfare. In 2012, for example, we have shown that early stress produces life-long and transgenerational modifications in behaviour, stress reactions and gene expression in chickens (Goerlich et al., 2012 in Hormones and Behavior).

The ethology lab has recently published part of the results from the fear selection study showing that Red Junglefowl selected for low fear of humans displays correlated responses in a number of other behaviour traits. The role of two genes, TSHR and ADRA2C in chicken domestication is also under study, since they have recently been found to carry a clear signature of selection. Anders Wirén successfully defended his PhD thesis entitled “Correlated selection responses in animal domestication: the behavioural effects of a growth QTL in chickens”.

The genetics lab has made important progress in their attempt to dissect complex behavioural and physiological traits using Quantitative Trait Locus experimental approaches. Their paper in PLoS Genetics (Johnsson et al., 2012, A sexual ornament in chickens is affected by pleiotropic alleles at HAO1 and BMP2, selected during domestication) received a lot of media attention and demonstrated how two genes that were responsible for increasing comb mass also increased egg production and bone allocation. This revealed at a genetic level how a sexual ornament (the comb) can have pleiotropic effects on other traits.

The personality lab has started working with the incorporation of the first LiU PhD student Josefina Zidar. Zidar and Løvlie published a paper in Animal Behaviour showing the behavioural responses to olfactory cues by domestic fowl.

The physiology lab continues the work on the mechanisms of fetal programming of cardiac growth and function. In collaboration with Dane Crossley at the University of North Texas the group has shown distinct differences in the mechanisms of cardiovascular regulation in different chickens breeds (Crossley and Altimiras, 2012 in Poultry Science). The group is also collaborating with Alvaro Garitano from Universidad Mayor de San Andrés in La Paz, Bolivia in the study of cardiac function in the Ornate Tinamou, a primitive bird that thrives in the Andean Altiplano at 4000 meters above sea level. To support the increasing need for studies in cellular models a new cell culture facility was installed and studies on the growth of cardiac cells in response to different hormones and environmental factors are being carried out.

Further information, news and publications from the AVIAN group can be found at http://www.ifm.liu.se/biology/zoology/avian/
Conservation Ecology Group

STAFF
Professors: Per Milberg

Research during 2012 focused on insect, trees, species-rich grasslands and deciduous forests.

We published a study on the saproxylic beetle fauna on old oaks (Quercus spp.) with the aim to find a spatial scale at which density of old oaks best explained the presence of species in a landscape. Finding such a spatial scale is important for conservation of biodiversity in oak-rich landscapes. Several projects with similar focus, but different approaches for sampling and analyses, are currently running.

In some of these spatial projects, we used a new pheromone-trapping method (where the males are attracted to a substance equivalent to the female pheromone). In 2012 we attempted two additional pheromone systems: a moth associated with large deciduous trees, and a group of moths in grassland (burnet moths), that are potential indicator species for monitoring biodiversity.

Another promising line of work involved species dependent on, or promoted by, forest fire.

Cooperation
Our projects involve cooperation with a number of universities and research institutes, e.g. University of Lund, Sweden; SLU (Uppsala, Alnarp, Umeå), Sweden; Mid Sweden University, Sweden; Oklahoma State University, USA; Middle Tennessee State University, USA; Haremaya University, Ethiopia; University of Ballarat, Australia.

External Activities
Monitoring of species is an important part of detecting environmental changes. Per Milberg, Lars Westerberg and Karl-Olof Bergman were involved in a national evaluation of monitoring programs in semi-natural grassland, and Per Milberg in a feasibility study for monitoring of agricultural weeds (both commissioned by the Board of Agriculture), and Lars Westerberg has an appointment as monitoring analysis expert (the Environmental Protection Agency). Karl-Olof Bergman is involved in a national monitoring program for biodiversity in semi-natural grasslands. Heidi Paltto has been invited to talk to staff members of authorities, and to give a course.

Our staff presented research for students and teachers from secondary schools in the county at the Popular Science Day, arranged by IFM. We have also been involved in presentations for the public arranged by the university, and have guided study visits from primary and secondary schools.

Highlights
Håkan Lättman presented his PhD thesis “Studies on spatial and temporal distributions of epiphytic lichens”. Heidi Paltto was promoted to docent (associate professor).

Since 2010 Kolmarden is engaged in the LIFE project SAMBAH (Static Acoustic Monitoring of the Baltic Harbour porpoise; www.sambah.org), which aims at, by using 300 passive acoustic data loggers, monitoring harbour porpoises in the Baltic Sea. Kolmarden is the international coordinator. The project is now in its second year of data collection; it will be completed in May 2013. The final report will be issued in December 2014.

Kolmården was also engaged in the 3-year EU-project, called EUZooS-XXI, (www.euzoos-xxi.org). It was finished in September 2012. It focussed on four important conservation topics: invasive alien species, endangered species, biological diversity and ecological connectivity. Representatives from the general public were invited and asked to produce concrete suggestions how these subjects could be presented to the zoo visitors. At

Many species of insects and fungi, including many rare ones, depend on forest fires. Preserving such species constitute a major challenge, and is likely to benefit from a landscape perspective.
Kolmarden this resulted in a new animal exhibit, called “Madagascar”, where three lemurs represented the island’s unique, critically endangered fauna. A rich variety of information was developed around the exhibit, e.g. via large touch screens and daily oral presentations by zoo educators.

Kolmården’s engagement in the LiU Masters program “Applied Ethology and Animal Biology” continues, with several course parts carried out in the zoo, e.g. the entire 7hp course Zoo Biology.

Josefin Starkhammar at the Division of Electrical Measurements, University of Lund, supervised by Mats Amundin, defended her doctoral thesis in the end of 2011. The final paper was published in the beginning of 2012. It presents a technical description of the multi-hydrophone system that she developed. The project was funded by the Research Council, and was called ELVIS (Echo-Location Visualization and Interface System).

Figure 1. The ELVIS system, with the 47-hydrophone matrix in front of a dolphin. In the acoustic “touch” screen configuration this screen is mounted in front of an underwater window, allowing the dolphins to see active symbols and the computer screen graphics projected on the screen.

REFERENCES


Plant Evolution and Domestication Group

STAFF
Associate Professor: Johan Edqvist, Jenny Hagenblad
Assistant Professor: Matti Leino
First Research Engineer: Kristina Blomqvist
Post doc: Hugo Oliveira
PhD student: Monica Malmbecker Edstam, Nils Forsberg
Technician: Maria Lundström, Tove Bjerg
Director of studies: Agneta Johansson

RESEARCH AND PHD TRAINING
The PlantED group focuses on two main lines of research. The LTP team headed by Johan Edqvist focuses on understanding lipid transport proteins using Physcomitrella patens and Arabidopsis thaliana as model systems. The Historic Seed Group, headed by Jenny Hagenblad and Matti Leino explores the evolution crop plants in a range of crop species cultivated in Scandinavia.

The research in the LTP group is focused on function, structure and evolution of the non-specific lipid transfer
protein (ns-LTP) in plants. The Historic Seed Group runs several projects concerning the genetics and evolution of landrace crops and agricultural history with particular attention to crops cultivated in Fennoscandia. Both genebank material and seed samples from historical collections are used for the studies and both neutral markers and functional genes are investigated to explore both population genetic structure and specific traits such as flowering time and nutrient content of historical crops.

In addition to the research the PlantED group has also run a bi-weekly journal club where also researchers and PhD students not in the PlantED group have joined to discuss the latest findings within plant genetic research.

HIGHLIGHTS
A number of new people have been recruited to the group: Kristina Blomqvist as First Research Engineer, Nils Forsberg as a PhD student and Hugo Oliveira as a post-doctoral researcher. The LTP group has established an efficient system for production of plant lipid transfer proteins. We have also identified novel Arabidopsis phenotypes showing a role for LTPs in seed development.

The Historic Seed Group has in collaboration with researchers at INRA Clermont-Ferrand published a world-wide screen of a nutrient content gene in wheat in Theoretical and Applied Genetics. An extensive screen of the genetics of landrace grey pea during the past century and a half has been published in Hereditiy. Two papers on genetic diversity on Mediterranean wheat have been published in PLoS One and Genetic Resources and Crop Evolution respectively. A Swedish language overview on the origin of hops in Sweden has been published in Svensk Botanisk Tidskrift, and a popular science essay on the history of the stem rust disease was published in Fataburen. The Historic Seed Group also hosted a meeting with two researchers from Cambridge, hopefully the initiation of future collaborations.

COLLABORATIONS
External collaborations
LTP group – Tiina Salminen (Åbo Akademi University), Peter Mattjus (Åbo Akademi University), Magnus Eklund (University of Melbourne)
Historic seed group – François Balfourier and Catherine Ravel (INRA Clermont-Ferrand, France), Robbie Waugh and Joanne Russell (James Hutton Institute, Scotland), Anna Palmé (NordGen, Alnarp), Linnéa Asplund (SLU, Uppsala), Else-Marie Strese and Per Larsson (Nordiska museet, Julita), Kristiina Antonius (MTT Agrifood Research, Finland), Jim Weller (University of Tasmania, Australia) and Bente Graae, Christophe Pelabon, Atle Bones and Torfinn Sparstad (Norwegian University of Science and Technology, Trondheim)

EXTERNAL ACTIVITIES
The Historic Seed Group has participated with talks and posters at five international meetings. The senior members of the group have also been evaluating a PhD dissertation, a PhD half-time report and an ERC advanced researcher grant application. The Historic Seed Group has also been represented at workgroup meetings at NordGen and the Swedish programme for diversity of cultivated plants (POM)

SPECIAL EVENTS
In May Jenny Hagenblad received a stipend from King Carl XVI Gustaf 50th Anniversary Fund for Science, Technology and the Environment from HRH Carl XVI Gustaf. In November Matt Leino was promoted “docent” in genetics.

The Sensory and Behavioral Physiology Group

STAFF
Professors: Matthias Laska

Research in the Sensory and Behavioral Physiology Group focuses on odor structure-activity relationships, that is, on determining the properties of stimulus molecules that are critical for the interaction with an olfactory receptor and thus for the odor quality they evoke. A second research topic concerns correlations between chemosensory performance and neurobiological and genetic properties such as the size of olfactory brain structures or the size of the olfactory receptor repertoire. With both topics, a comparative approach including human subjects and a variety of animal models is employed.

HIGHLIGHTS
Matthias Laska and one of his students were able to demonstrate that mice are extraordinarily sensitive to the odor of aliphatic carboxylic acids, substances known to be part of their body odor. The mice detected concentrations as low as 3 ppt (parts per trillion) and displayed significant correlations between olfactory sensitivity and molecular structural features of the odorants such as length or branching of the carbon chain (Güven and Laska 2012. PLoS ONE 7: e34301).
In collaboration with the Centre for Research in Animal Behaviour at the University of Exeter (England), Nellie Linander showed that honeybees are able to detect the odor of amino acids, important constituents of floral nectar, at millimolar concentrations (Linander, Hempel de Ibarra, and Laska 2012. Chem. Senses 37: 631-638).

Josefin Arvidsson succeeded in training the Asian elephants at Kolmården zoo to cooperate in a food-rewarded olfactory discrimination test, thus adding yet another species to the comparative studies on olfactory performance performed by the group. She found that elephants are even faster than dogs, mice, and rats in learning new olfactory tasks (Arvidsson, Amundin, and Laska 2012. Physiol. Behav. 105: 809-814).

In collaboration with the Instituto de Neuro-Etologia of the Universidad Veracruzana (Mexico), Pia Katrine Løtvedt demonstrated that spider monkeys are highly sensitive to the typical “green odors” emitted by young leaves. Further, she found that the number of functional olfactory receptor genes are poor predictors of olfactory sensitivity in primates (Løtvedt, Murali, Hernandez Salazar, and Laska 2012. Pharmacol. Biochem. Behav. 101: 450-457).

Master’s student Josefin Arvidsson training Asian elephants in an olfactory discrimination test at Kolmården Wildlife Park

COOPERATION.
The Sensory and Behavioral Physiology Group has a long-standing collaboration with the Instituto de Neuro-Etologia of the Universidad Veracruzana in Xalapa, Mexico. Every year, students enrolled in the International Master’s Program “Applied Ethology and Animal Biology”, have the possibility to perform the experimental part of their thesis work in Mexico and collect data on chemosensory performance in spider monkeys. The group is also collaborating with the Department of Food Chemistry at the University of Erlangen, Germany, where joint studies on the chemical composition of complex natural odors are performed. The group is also collaborating with the Department of Neurobiology at Yale University in New Haven, Connecticut, and is involved in a joint project on the phenotypical characterization of Alzheimer’s disease model mice. Further, the group is collaborating with the Centre for Research in Animal Behaviour at the University of Exeter, England, in a joint project on comparative olfactory performance in honeybees and mammals. Finally, the group is collaborating intensively with Kolmården Wildlife Park where numerous studies are performed.
The research branch of Chemistry, cover all traditional areas of chemistry. The major research programs Protein Chemistry, Molecular Biotechnology and Organic Chemistry all have a strong focus on Molecular Life Science and Chemical Biology. Research activities in Analytical Chemistry, Inorganic Chemistry and Physical Chemistry are led by senior staff, often in cooperation with other researchers in the department and with other research programs at the University.

In parallel we are also screening conditions to crystallize the proteins ultimately misfold into cross-beta-sheet structure of amyloid fibrils. The central image is a transmission electron micrograph of lysozyme amyloid fibrils taken at 80000 fold magnification.

THIOPURINE METHYLTTRANSFERASE (TPMT) is a polymorphic enzyme and a key enzyme in treatment of childhood leukemia and inflammatory bowel diseases such as Crohn’s disease. TPMT is one of the few classical examples of pharmacogenetics where the dosages of medical drugs are directly dependent on the polymorphism of the enzyme.

In collaboration with Department of Clinical Pharmacology at University Hospital in Linköping mutants of different variants are engineered and biophysically characterized, using a repertoire of techniques such as enzyme activity measurements, circular dichroism, fluorescence and differential scanning calorimetry.

In parallel we are also screening conditions to crystallize the various variants.
PROTEIN-PROTEIN INTERACTIONS are intrinsic to virtually every cellular process. We are studying the interaction of the cellular receptor tissue factor (TF) with the coagulation factors VII (FVII) and X (FX) that is the key step in the initiation of blood clotting and thrombus formation. The information output from this project will directly be used in drug design of therapeutic agents that can intervene in the association process of FVII and FX to TF.

Molecular Biotechnology

STAFF
Professors: Bengt-Harald "Nalle" Jonsson, Maria Sunnerhagen
Assistant Professors: Patrik Lundström, Martin Karlsson
Associate Professor: Ann-Christin Brorsson
Post-docs: Lotta Tegler, Cecilia Andrésten, Theresa Lindholm
PhD students: Cecilia Andrésten, Anna-Lena Göransson, Jutta Speda, Linda Helmforss, Sara Helander, Alexandra Ahlner, Annica Blissnig, Madhan Anandapadmanabha, Mikaela Eliasson
Administrator: Susanne Andersson

ACTIVITIES
The research activities in molecular biotechnology are focussed on detailed characterizations of protein structure and dynamics at the molecular level. The role of protein interactions for understanding a variety of biological functions are addressed in different projects. The results which are gleaned from our studies of these fundamental biological phenomena are also utilized in projects, which aim at efficient diagnosis and novel strategies for treatment of some human diseases.

THE PROTEIN MISFOLDING DISEASE ALS: The mis-folding and intracellular aggregation of the protein superoxide dismutase is strongly coupled to the neurodegenerative disease ALS. To find the molecular basis for ALS we perform a detailed characterization of the structural and dynamical effects of a large set of different ALS-associated mutations in the gene for CuZnSOD. Therefore, we have used chemical cross-linking, analytical ultra-centrifugation and hydrogen/deuterium-exchange experiments to unravel the effects of the mutations on the dynamics of the protein.

PROTEIN-SURFACE INTERACTIONS. Enzymes are of increasing use in biotechnological applications. Regardless of the application, the enzymes will always encounter surfaces and this will often lead to that the enzyme activity is lost. It has been a long standing perception that "soft" proteins are proteins that bind to, and unfolds at, surfaces even when there are no apparent attractive force between the protein and the surface. There is however little knowledge about which features of a protein that dictates whether a protein will behave as a "soft" protein or a "hard" protein, although the physical stability of the protein is believed to play a crucial part. In order to discriminate between the importance of thermodynamic stability and kinetic stability we have engineered protein variants with these properties separated. Our aim is to pinpoint which feature is the most important so that the correct modifications can be performed on proteins that are to be used in various biotechnological applications.

STABILIZATION OF CARBONIC ANHYDRASE. At this time there is a consensus view that the concentration of CO2 in the atmosphere is the major contributor to increasing global warming and much effort is directed to find methods for carbon capture and sequestration (CCS). However, no method has thus far proved to be practically or economically feasible. Since the natural function of carbonic anhydrases is to facilitate the removal of carbon dioxide from the blood it has been suggested that carbonic anhydrases can be used as biological catalysts in bioreactors designed for capturing CO2 from various gas streams. However, there are no naturally occurring carbonic anhydrases that have high enough stability to be used in such a bioreactor. We are therefore currently working on the design of engineered human carbonic anhydrases with increased stability which can then be used as catalysts in enzyme based bioreactors for carbon capture and sequestration.

FUNCTIONALIZATION OF NANOPIXRTICLES BY PEPTIDE DESIGN: Earlier studies have given us a firm knowledge about the structure of and dynamics in proteins upon adsorption to solid surfaces. Recently we have unraveled fundamental principles that govern the formation of helical structure on silica nanoparticles, which is important in the development of devices that interact with biological systems.

ALZHEIMER'S DISEASE: The aim of this project is to perform detail studies of the molecular origins of Alzheimer’s disease (AD). The aggregation process of the amyloid β peptide (associated with AD) is studied by using Drosophila melanogaster as a model organism, in parallel with biophysical studies. The challenge is to identify and characterize toxic species as well as to study the influence of cellular factors on the toxicity. This knowledge will then be used to test the effect of anti-aggregation agents in vitro as well as in vivo.

LYSOZYME AMYLOIDOSIS: Misfolding and aggregation of lysozyme are associated with lysozyme amyloidosis where abnormal depositions of aggregated protein are found in organs such as the liver, spleen and kidney. By expressing lysozyme in Drosophila melanogaster we can study the aggregation of these proteins in a complex multicellular environment and look into the role of specific cellular factors and pathways in the pathogenesis caused by lysozyme misfolding and aggregation. Results from studies using this Drosophila model suggest that the onset of familial amyloid disease is linked to an inability of the quality control system in the cell to completely degrade the amyloidogenic lysozymes prior to secretion, resulting in secretion of these destabilised variants, thereby leading to deposition and associated organ damage.

RATIONAL ENZYME MINING: Enzymes are biological catalysts that find their use in a large number of biotechnological applications and enzyme based industrial processes are expected to increase in the near future. One central concern in order to realize the promise of industrial biotechnology is then to find new enzymes that are active and stable at the conditions of interest. In this respect microorganisms are an ideal source of novel enzymes since they can survive and propagate in many environments. However, to be able to screen full microbial communities for new enzymes methods that is independent of pure culturing needs to be developed. We are currently working on the development of such methods to mine for new enzymes in methanogenic microbial communities in experimental biogas reactors.
ENZYMATIC ENHANCEMENT OF SLUDGE DIGESTIBILITY: As partners of the centre of excellence in biogas research, recently established at LiU with support from the Swedish Energy Agency, we are investigating the possibilities to enhance sludge digestibility with enzymes for increased biogas production. The aim of the research is to determine whether enzyme addition de facto is a feasible method to increase biogas production. For this, it is necessary to monitor the fate of added enzymes by determining the activity, modification and lifetime of each type of added enzyme at the conditions that would prevail in a real life process, rather than simply observing the effect in biogas production. This can then be used to correlate enzyme activity to e.g. metabolite turn-over and possible inactivation mechanisms of added enzymes. This will also give information about e.g. which of the many commercially available enzymes which are the most suitable for the intended process.

BACTERIAL AND IMMUNOLOGICAL RESPONSES IN INFECTIOUS DISEASE. The human Ro52 protein is an autoimmune target in Sjögren’s disease, and involved in the production of fetal antibodies in pregnant mothers. We have characterised the interaction of the disease-related antibodies and are currently characterising the subdomains of Ro52 and their interactions on a molecular level.

Our most recent results show that patient autoantibodies that hinder ubiquitination interfere with the E2-binding surface of the E3-active RING domain of Ro52. Taken together with our previous studies, we can now propose an action model for the entire Ro52 protein (Fig III, below) MexR is a DNA-binding protein that regulates the expression of the Pseudomonas Aeruginosa efflux pump, and a target for antibiotic resistance mutations leading to multi-drug resistance. We have described the biophysical and molecular basis for resistance and are currently evaluating their implications on structure.

Globule structure, perhaps a prerequisite for its high-affinity binding to a range of biologically important target proteins. A range of protein interactions are currently being screened on a structural level.

STRUCTURAL BIOLOGY IN CANCER AND INFECTIOUS DISEASE The group of Maria Sunnerhagen is currently describing a series of intrinsically disordered interactions between the c-Myc trans-activating domain and its regulatory co-partners, including Bin1 and TBP, using both NMR and crystallography. The Ro52/Trim21 regulatory network including E2 ligases Ubch6 and Ubch8 is addressed using a range of biophysical and biochemical techniques. In our Pseudomonas Aeruginosa project, aimed to investigate principles for novel antibiotics, several novel protein structures have been determined and molecular dynamics simulations reveal novel principles for how mutations result in antibiotics resistance.

REGULATION OF KINASE ACTIVITY. Eph proteins are involved in developmental processes such as cell migration, angiogenesis and axon guidance and in the adult organism they have been implicated in certain cancers. The crystal structure of the kinase domain of EphB2 as well as those of other Eph proteins suggests that the ground-state cannot be catalytically active. Our working hypothesis is that a low-populated “excited” state is responsible for catalysis and we have shown that the protein exchanges between the ground-state and something else on the millisecond time-scale. We are currently using NMR spectroscopy and x-ray crystallography to further study the interplay of structure and dynamics for this unusual mode of enzyme regulation.

Organic Chemistry

STAFF
Professors: Peter Konradsson, Ingemar Kvarnström
Associate professor: Stefan Svensson
Assistant professor: Peter Nilsson
Senior researcher: Åsa Rosenquist
Post-doc: Marcus Bäck, Anders Dahlgren, Hamid Shirani
Technician: Mikaela Eriksson
Administrator: Susanne Andersson

ACTIVITIES
Synthesis of functionalized oligothiophene derivatives with specific optical and electronic properties: By combining the features of polymers and the electro-optical properties of conjugated molecules, conjugated polymers suitable for a wide range of applications, such as solar cells, displays and biosensors are created. Our research is mainly focused on creating well-defined oligothiophene derivatives through rational chemical design (See figure below, and highlight) As a first instance we are synthesizing oligothiophenes that can
be utilized as tools for studying biological and pathological processes. The aim of these projects is to provide molecular tools that can be used for real-time imaging of biological events from the nanoscopic level (biomolecules and cells) to the macroscopic level (organs and body). Secondly, we are also investigating if similar molecular scaffolds can be utilized as therapeutic active agents towards distinct pathological processes. Furthermore, we are developing electro-active oligothiophene derivatives that can be combined with defined biological templates, such as amyloid fibrils, to generate materials that can be implemented in research areas such as nanobioelectronics. Though a multidisciplinary collaboration with other researchers at IFM and ITN, we are aiming at developing novel materials that can be used for electronic release of pharmacueticals, and devices that can stimulate and record cellular activity in complex environments.

**SYNTHESIS OF POTENTIAL PROTEASE INHIBITORS:** Proteases are enzymes capable of restructuring peptides and proteins by specific hydrolysis and are therefore powerful mediators for health and disease. There are five different classes of proteases, classified according to the most significant functional group in the active site of the enzyme. Design and synthesis of inhibitors and screening for efficient and selective inhibitors of key proteases have become an attractive and powerful course for new drug development. This is an area of fundamental importance to the pharmaceutical industry. Structure-based drug design has been used in the search for potent and selective drug candidates. An important part of this is to find the minimum necessary chemical features for binding to a particular protease. Methods for screening of potential inhibitors are available and it is possible to screen large libraries of single compounds to identify lead compounds. Design and synthesis of inhibitors have been studied against the following proteases: HIV-1 protease, Hepatitis C protease, Malaria parasite proteases, Thrombin and γ-Secretase (Alzheimer’s disease). The research projects are done in collaboration with the University of Stockholm, BMC, Uppsala and Medivir AB, Huddinge.

**Fig IV:** General chemical structure of functionalized oligothiophene derivatives.

**Fig V:** A self-assembled monolayer (SAM) of MPTMS on a ZnO surface.
Inorganic Chemistry

STAFF:
Professor: Per-Olov Käll
Assistant Professor: Fredrik Söderlind
Associate Professor: Henrik Pedersen

ACTIVITIES
The research in inorganic chemistry at IFM is mainly focused on colloidal synthesis and characterisation of (i) magnetic metal oxide nanoparticles (e.g. Gd2O3) for magnetic resonance imaging; (ii) chemical or electrochemical synthesis of semiconducting nanoparticles, e.g. ZnO, CuO, Cu, as sensing material in gas sensing studies, e.g., of O2, NOx, CO, H2, MeOH. The above projects are pronounced interdisciplinary with collaboration partners both within and outside IFM.

(i) Several of the rare earth metals are strongly magnetic and at least one of them, gadolinium, is a unique because it combines a high magnetic moment with a very high cross-section for thermal neutrons, implying that Gd(III) containing nanocrystals are potentially interesting both as contrast agent in magnetic resonance imaging (MRI) and neutron capture therapy (NCT). We have found that small nanocrystals of cubic Gd2O3 produce significantly shorter T1 relaxation times than the conventional gadolinium containing chelates normally used in examination of patients. A possible explanation of the effect is the higher density of magnetic active ions in a nanoparticle compared to that of a bulky chelate providing access of only a single water molecule to the magnetic central atom.

(ii) A novel sensing project carried out in collaboration with Profs. Anita Lloyd-Spetz and Lars Ojamäe is the development of a SiC based methanol sensor for application under demanding conditions. Two articles have so far been published in Sensors and Actuators: Chemical where Pt and Ir have been tested as sensing materials.

(iii) During the year, a new project has been started in collaboration with Profs. Magnus Odén at the Div. of Nanostructured materials, and Lars Ojamäe at Physical chemistry. The project which is partly funded by KAW aims at the experimental and theoretical study of catalytic hydrogenation of CO2 in the formation of methanol or dimethyl ether. So far a high pressure reactor (autoclave) and a GC has been installed, an MS to be connected with the GC presently being under purchase (see fig VI)

Analytical Chemistry

STAFF
Professor: Elke Schweda
Associate Professor: Johan Dahlén

ACTIVITIES
Research in Analytical Chemistry is focused on analytical carbohydrate chemistry and studies structures of biologically active carbohydrates from pathogenic bacteria. Of particular interest are the exclusively human pathogen non-typeable Haemophilus influenzae (NTHi) and Helicobacter bizzozorii, which normally colonizes cats and dogs. Humans potentially acquire gastric infections as a consequence of direct contact with these animals. NTHi causes otitis media and both acute and chronic lower respiratory tract infections in small children. The potential of both NTHi and H. bizzozorii to cause disease depends upon their surface expressed carbohydrate antigen, lipopolysaccharide (LPS).

The heterogeneity and structural complexity of LPS from pathogenic bacteria pose significant analytical challenges. Typically, structural profiling involves analyses by chemical, nuclear magnetic resonance (NMR) and mass spectrometric (MS) methods. Electrospray ionization mass spectrometry (ESI-MS) has played an increasingly important role in the characterization of LPS.

CHEMISTRY-HIGHLIGHTS
I. Johan Dahlén has been appointed associate professor in analytical chemistry

II. Henrik Pedersen has been appointed associate professor in inorganic chemistry

III. A study from the Hammarström lab in collaboration with the Nilsson and Thor labs showed that Curcumin, a substance extracted from turmeric, prolongs life and enhances activity of fruit flies with a nervous disorder similar to Alzheimer’s disease.
Alzheimer’s disease, which is characterized by the accumulation of sticky amyloid-beta and Tau protein amyloid fibrils. Linköping researchers wanted to investigate how the substance affected transgenic fruit flies (Drosophila melanogaster), which developed evident Alzheimer’s symptoms. Flies showed enhanced activity, deceased neurotoxicity and lived up to 75% longer when treated with curcumin. However, surprisingly the amount of amyloid in the brain or eyes did not decrease. Curcumin did not dissolve the amyloid plaque; on the contrary it accelerated the formation of mature fibrils by reducing the amount of their precursor forms, known as oligomers.

The study hence, indicates that it is the initial stages of fibril formation and fragments of the amyloid fibrils that are most toxic to neurons and that curcumin accelerated this conversion step.


IV. A study from Nilsson lab in collaboration with Hammarström and with colleagues at the University Hospital in Zürich (Aguzzi) tested luminescent conjugated polymers, or LCPs, on organotypic live tissue sections from the brains of mice that had been infected with prions. The results show that the number of prions, as well as their toxicity and infectibility, decreased drastically. This is the first time anyone has been able to demonstrate the possibility of treating illnesses such as “mad cow” disease and Creutzfeldt-Jacobs with LCP molecules. The course of prion disease is relentless when the prions fall to pieces and replicate at an exponential rate. When researchers inserted the LCP molecules into their model system, the replication was arrested, through stabilizing the prion aggregates – which is a new concept in treating prion disease.


V. Elke Schweda and coworkers has characterized the structural diversity of the lipopolysaccharide from two Haemophilus influenzae strains. Vitiazeva V et al in Carbohydrate Res 357(2012) 98-110

VI. In a study by Annika Lenz, Lars Ojamäe and coworkers from FOI and Lund University the reaction mechanism of DNT decomposition on platinum nanoparticles was elucidated. This is of importance for understanding the detection of explosives by chemical sensors.


VII. Lars Ojamäe and Per-Olov Käll are members of the “Designed Nanoparticles” project that was awarded a major grant from the Knut and Alice Wallenberg Foundation. They will study the catalytic conversion of carbon dioxide to methanol by the use of novel nanoparticles. A new PhD student in physical chemistry will be enrolled in the project in 2013.

VIII. Yuan Liu obtained a grant from the China Scholarship Council to join Lars Ojamäe’s group as a PhD student, which he did in October 2012. His studies will focus on CH4 and CO2 ice clathrate structures and their implications for atmospheric chemistry and for carbon dioxide storage.
SCIENTIFIC BRANCH OF
Material Physics

GENERAL INFORMATION

STEERING COMMITTEE
Lars Hultman (Head), Erik Janzén (Deputy Head), Weimin Chen, Ulf Helmersson, Magnus Odén, and Roger Uhrberg.

RESEARCH DIVISIONS AND PROFESSORS

Functional Electronic Materials: Weimin Chen, Head
Irina Buyanova

Nanostructured Materials:
Magnus Odén, Head
Bo Jansson (Adjunct SECO Tools AB, deceased)

Plasma and Coatings Physics:
Ulf Helmersson, Head
Nils Brenning (Adjunct from KTH, Stockholm)

Semiconductor Materials:
Erik Janzén, Head
Peder Bergman
Anne Henry
Per-Olof Holtz
Leif Johansson
Rositza Yakimova (Emerita)
Bo Monemar (Emeritus)

Surface and Semiconductor Physics:
Roger Uhrberg, Head
Göran Hansson (Prefect of IFM)
Wei-Xin Ni

Thin Film Physics:
Lars Hultman, Head
Jens Birch, Deputy Head
Esteban Broitman (Guest Prof. Carnegie-Mellon)
Joseph E Greene (Guest Prof., Univ. Illinois)
Ivan Petrov (Guest Prof., Univ. Illinois)
Michel Barsoum (Guest Prof., Drexel Univ.)

INDIVIDUAL AND COORDINATED EXCELLENCE RESEARCH PROGRAMS

Government Strategic Grant (SFO) for Materials

- ERC Advanced Grant (Hultman)
- ERC Starting Grant (Rosén)
- KAW Project Isotopic Control - Ultimate Properties (Janzén, Hultman, Greene, Abrikosov)
- KAW Scholar Grant (Hultman)
- KAW Academy Fellow (Rosén)
- ESF Epitaxial Graphene EPICRAT (Janzén et al)
- EDA/FMV GaN HEMT MANGA (Janzén et al)
- EU EuSiC (Janzén et al)
- VR Linnaeus Center LiLi-NFM (Hultman et al)
- VR/RAC Coordinated Program Grant Materials Science using High-Energy X-Rays (Birch et al)
- VR SiC Material for Power electronics (Janzén)
- VINNEX Center FunMat (Hultman et al)
- Nordic Research Center SIMARC (Chen et al)
- SSF Coordinated Grant in Materials Science MultiFilms (Odén et al)
- SSF Nano-N (Holtz et al)

- SSF Synergy Grant FUNCASE (Hultman et al)
- SSF project: III-nitrides for UV and high frequency applications (Janzén et al)
- SSF project: SiC – the Material for Energy-Saving Power Electronics (Janzén et al)
- The Linköping Center for Nanoscience & Nanotechnology CeNano (Hultman, Chair)
- FP7 EU project: Nano-RF (PI R. Yakimova)

SUMMARY OF ACTIVITIES

The Material Physics Area is the largest research unit of the Faculty and is internationally recognized as a strong research environment. It engages ~150 persons, including over 60 PhD students.

The research is of a basic experimental character, but direct collaboration with industry is essential in many projects. Theoretical modelling is a natural part of many projects.

The research activities include growth of a variety of material structures with different techniques, mainly PVD, CVD and sublimation-based. The materials studied span a broad field, such as metallic thin films, semiconductor materials, nanostructures, and organic structures.

We operate several advanced laboratories; mostly in clean room environment. The characterization techniques include electron microscopy (SEM, TEM, FIB, EELS, PL, CL) and surface studies (ARUPS, STM, AFM, XRR, ERDA, XPS), partly at external synchrotron radiation facilities, but also extensively optical, transport and magnetic resonance techniques. Collaboration with foreign laboratories is typical for all research groups; in fact most published papers have international co-authors.

EDUCATION

In 2012, 11 PhD theses were published in our divisions.

The researchers are heavily involved in teaching on the basic and advanced level in physics, materials science, and nanotechnology (>10 courses). ~10 courses for PhD students are also given each year.

Prof P O Holtz is Director of the Graduate Education at IFM including the Graduate School in Materials Science: AGORA Materiae.

Prof. I I Johansson retired as Director of the Master Education in Materials Physics at LiTH and Director for undergraduate teaching in Physics at IFM in 2012.

We are host for the EC Erasmus-Mundus graduate school for Material Science and Engineering DocMase (Odén et al).

Lars Hultman won the Junior Faculty Prize 2012 at LiU for supporting the careers of junior researchers, thus creating a sustainable research environment.

TECHNOLOGY TRANSFER & PUBLIC INTERACTION

Dr Galia Pozina won the IVA – Royal Swedish Academy of Engineering Sciences ”Mentor 4Research” Prize – a catalysts for Commercialization.

Our research has generated high-tech industries like Norstel AB in Norrköping, producing SiC substrates, Epigress AB in Lund, producing SiC growth systems, and Impact Coatings AB in Linköping, developing PVD-processes and equipment for functional and decorative thin films. A spin-out company Cyclops AB develops a novel SiC epitaxial tool.

We are also part of the LiU Fund Raising Campaign; www.liu.se/expanding_excellence.

Several patent applications were filed in 2012.

HIGHLIGHTS 2012

Linköping University is taking part in the Graphene Flagship ramp-up stage, which is funded by EC within the FP7, to bring
this amazing material to revolutionary solutions in high speed electronics, medical diagnostics, space research, etc. Researchers at IFM have the know how to produce the best graphene on silicon carbide world wide. A goal of the Graphene Flagship is to bridge research and commercialization by creating new and improved graphene products to be implemented in advanced applications, which will bring value to the society. The first European company on epitaxial graphene (Graphensic AB) is operated out of Linköping.

We have experimentally demonstrated the first spin amplifier operating at room temperature - one of the fundamental building blocks in spintronics. This defect-engineered spin amplifier is based on a non-magnetic semiconductor Ga(In)NAs, with a large spin gain (> 2700% at zero field) and a high cut-off frequency (> 1 GHz).Adv. Mater. 25, 738 (2003)

We reported on the Magnetic quantum ratchet effect in graphene. Orbital effects in the presence of an in-plane magnetic field provide strong evidence for the existence of structure inversion asymmetry in graphene. Nature Nanotechnology 8, 104–107 (2013)

In the area of ZnO-based materials, several topics were addressed. We have continued our studies of exciton dynamics and exciton-photon coupling in bulk and nanostructured ZnO. We have also initiated investigations of non-linear optical and plasmonic effects in ZnO NWs. In bulk ZnO, signatures of excitons bound to isoelectronic centers - an important class of excitons and defects that have so far hardly been investigated in ZnO, were provided. Impact of various intrinsic defects on p-type doping of ZnO via ion implantation with phosphorous and nitrogen were also examined.

In 2012, we have conducted detailed studies of spin-dependent properties of self-assembled InAs/GaAs QD, QD molecules and rings. Special attention was paid to understanding the physical mechanism for spin injection, spin relaxation and spin detection.

For dilute nitrides like Ga(In)NAs and Ga(Al,Ga)NP, the presence of harmful residual defects is still one of the major obstacles preventing the materials from practical applications in photonics and optoelectronics. In 2012, we have continued our experimental efforts to identify point and interfacial defects that are responsible for deteriorating optical quality of the materials. We have also initiated new research activities on GaP/GaNP core/shell NWs. Great potential of these structures as nano-sized light emitters was demonstrated based on the observation of intense emission from a single NW at room temperature. Our current efforts are devoted to improving optical efficiency of the NWs via optimization of their structural design and material quality.

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We have also been actively involved in the education program for undergraduate students. During the year, the courses in “Semiconductor Technology” (TFYA39) and “Perspectives on Physics” (TFFM12) were given.

STAFF
Professors: Weimin Chen, Head of Division
Irina Buyanona
Post-docs and visiting scientists (>1 month): Daniel Dagnelund,
Jan Stehr, Alexandr Dobrovolsky, Galyna Rudko, Igor Vorona
PhD students: Jan Beyer, Shula Chen, Stanislav Filippow,
Yuttapoom Puttisong
Administrative/Technical staff: Susanne Andersson,
Anna-Karin Stål, Arne Eklund

SUMMARY OF ACTIVITIES
We conduct scientific research on electronic, magnetic and optical properties of semiconductor materials and nanostructures. The materials systems under study in 2012 include: (i) advanced spintronic materials based on II-VI and III-V semiconductors;
(ii) ZnO-based materials and nanostructures; (iii) self-assembled InAs/GaAs quantum dot (QD) nanostructures; (iv) dilute nitrides; and (v) GaP/GaNP core/shell nanowires (NWs). The research has been carried out mostly through close collaborations with many groups worldwide. Our aim is to obtain a better understanding of fundamental physical properties and a good control of materials properties, and to fully explore functionality of the studied materials for applications in future generation micro- and nano-electronics and photonics, spintronics, as well as in potential multifunctional devices and systems.

In the area of spintronic semiconductors, we have continued and extended studies of our recently discovered room temperature spin-filtering in a non-magnetic semiconductor Ga(In)NAs. The focus has been on development of room-temperature spin amplifier and spin detector based on Ga(In)NAs. We have also studied magnetic interactions in coupled CdSe/ZnMnSe QD structures.

Fig.1 A schematic picture of the demonstrated defect-engineered spin amplifier.

EVIDENCE FOR COUPLING BETWEEN EXCITON EMISSIONS AND SURFACE PLASMON IN Ni- COATED ZNO NWs
We show that coating ZnO NWs with a transition metal, such as Ni, can increase the efficiency of light emission at room temperature. Based on detailed structural and optical studies, this enhancement is attributed to energy transfer between near-band-edge emission in ZnO and surface plasmons in the Ni film which leads to an increased rate of the spontaneous emission. It is also shown that the Ni coating leads to an enhanced non-radiative recombination via surface states, which becomes increasingly important at low measurement temperatures and in annealed ZnO/Ni NWs. [Nanotechnology 23, 425201 (2012)]
DYNAMIC NUCLEAR POLARIZATION AND ITS EFFECT ON ELECTRON SPIN RELAXATION AND DEPHASING IN INAS/GAAS QDS

Electron spin dephasing and relaxation due to hyperfine interaction with nuclear spins is studied in an InAs/GaAs QD ensemble as a function of temperature up to 85 K, in an applied longitudinal magnetic field. The extent of hyperfine-induced dephasing is found to decrease, whereas dynamic nuclear polarization (DNP) increases with increasing temperature. We attribute both effects to an accelerating electron spin relaxation through phonon-assisted electron-nuclear spin flip-flops driven by hyperfine interactions, which could become the dominating contribution to electron spin depolarization at high temperatures. [Appl. Phys. Lett. 100, 143105 (2012)]

MECHANISM FOR RADIATIVE RECOMBINATION AND DEFECT PROPERTIES OF GAP/GANP CORE/SHELL NWs

Recombination processes in GaP/GaNP core/shell NWs grown on a Si substrate by molecular beam epitaxy are examined using a variety of optical characterization techniques, including cw- and time-resolved photoluminescence (PL) and optically detected magnetic resonance (ODMR). Superior optical quality of the structures is demonstrated based on the observation of intense emission from a single NW at room temperature. This emission is shown to originate from radiative transitions within N-related localized states. From ODMR, growth of GaP/GaNP NWs is also found to facilitate formation of complex defects containing a P atom at its core that act as centers of competing recombination. [Appl. Phys. Lett. 101, 143105 (2012)]

SUB-MILLISECOND DYNAMIC NUCLEAR SPIN HYPERPOLARIZATION IN A SEMICONDUCTOR: A CASE STUDY FROM PIn ANTISITE IN InP

ODMR is employed to identify key factors governing DNP in a semiconductor. We demonstrate that the extent of DNP can be efficiently controlled by varying lifetime of the localized electrons that transfer spin angular momentum to nuclei. The ultimate speed of a DNP process, on the other hand, is determined by the strength of hyperfine interaction that drives DNP. We show that about 50% nuclear spin polarization of a PIn antisite in InP can be achieved by shortening electron lifetime within a remarkably short time (<0.1 ms), see Fig.2, due to strong hyperfine coupling. [Phys. Rev. B 86, 205202 (2012)]

EFFICIENT UPCONVERSION OF PHOTOLUMINESCENCE VIA TWO-PHOTON-ABSORPTION IN BULK AND NANOROD ZNO

Efficient upconversion of PL from donor bound excitons is revealed in bulk and nanorod ZnO and attributed to two-photon-absorption (TPA) and two-step TPA (TS-TPA) processes. The TSTPA process is found to occur via a defect/impurity (or defects/impurities) with an energy level (or levels) lying within 1.14-1.56 eV from one of the band edges, without involving photon recycling. One of the possible defect candidates could be VZn. A sharp energy threshold, different from that for the corresponding one-photon absorption, is observed for the TPA process and is explained in terms of selection rules for the involved optical transitions. [Appl. Phys. B: Lasers and Optics 108, 919 (2012)]

ZEEMAN SPLITTING AND DYNAMICS OF AN ISOELECTRONIC BOUND EXCITON NEAR THE BAND EDGE OF ZNO

Comprehensive time-resolved PL and magneto-optical measurements are performed on a bound exciton (BX) line peaking at 3.3621 eV (labeled as I*). Though the energy position of I* lies within the same energy range as that for donor bound exciton (DX) transitions, its behavior in an applied magnetic field is found to be distinctly different from that observed for DXs. An exciton bound to an isoelectronic center with a hole-attractive local potential is shown to provide a satisfactory model that can account for all experimental results of the I* transition. [Phys. Rev. B 86, 235205 (2012)]

COLLABORATIONS

We have active scientific cooperation with over 20 international groups, including an on-going exchange program sponsored by the Swedish Institute through the Visby program (Inst. of Semiconductor Physics, Ukraine, and A.F. Ioffe Physico-Tehnical Institute, Russia).

Nanostructured Materials

STAFF

Professors: Magnus Odén, Bo Jansson*
Assistant Professors: Naureen Ghafoor, Mats Johansson Jöesaar, Fredrik Söderlind
Post-docs: Klara Asp Grönhagen, Mohamed Ballem, Lina Rogström
PhD students: Emma Björk, Axel Knutsson, Mohamed Ballem, Jennifer Ullbrand, Rickard Forsén, Niklas Norrby, Torkel Stenqvist, Robert Pilemalm, Susanne Sveen, Nina Shulumba, Isabella Schramm, Jenifer Barriero, Kumar Yalamanchili, Jing Yang, Aylin Atakan, Syed Bilal
Diploma students: Hassan Naureen
Administrative and Technical staff: Therese Dannetun, Karl-Olof Brolin

* Died Feb 2012
GENERAL INFORMATION
The division of Nanostructured Materials was established 1 April 2007 as a response to several research centers being granted at that time (i.e. Vinnova-FunMat, VR-LiLi-NFM, and SSF-MS2E). In 2009 SSF granted the group an additional Material Science program called MultiFilms and 2010 an Erasmus-Mundus graduate school, DocMase, with support from EC for 20 students was added. Naturally most of the Nanostructured Materials group’s research activities are related to these centers and programs.

The scientific aim of the group conforms to the material science paradigm: understanding of the synthesis, microstructure evolution, and material properties of nanostructured materials of industrial interest.

RESEARCH PROGRAMS

Hard coatings:
The thermomechanical properties of nanostructured reactive arc evaporated ceramic materials are studied in model systems that include a miscibility gap. Special interest is paid to the kinetics of the decomposition process in hard coatings and how it is influenced by the environment. Here we use high energy SAXS, and DSC as tools in situ study the formation of nm-sized particles within the solid solution. STEM and 3D-atom probe in combination with phase field and ab-initio calculations are used to further advance the understanding. An example of a reconstructed 3D-atom probe image of a multilayer is given in the figure below, i.e nanocandy.

In addition the microstructure evolution of alloyed cathode surfaces are also studied.

Mesoporous materials:
Synthesis of several types of pore structures with a variable pore size (30-300 Å) based on micelles and how to use these mesoporous materials as chemical microreactors. Of special interest is to use these frameworks to synthesize nanoparticles with narrow size distributions.

Engineering materials:
Application based research on surface behavior related to tribology at elevated temperature and brazing.

SCIENTIFIC HIGHLIGHTS

Two PhD graduated:
Lina Rogström: “High temperature behavior of arc evaporated ZrAlN and TiAlN films”
Axel Knutsson: “Thermal stability and mechanical properties of TiAlN-based monolithic and multilayer coatings”

Three Licentiate theses defended:
Niklas Norrby: “High pressure and high temperature effects of TiAIN”
Rikard Forsén: “Mechanical properties and thermal stability of arc evaporated Ti-Cr-Al-N coatings”
Jennifer Ullbrand: “Phase field modeling of spinodal decomposition in TiAIN”

Discovered surface directed spinodal decomposition in TiAIN, see figure, where a compositional wave originates at internal interfaces.

The influence of growth conditions and chemical composition on ZrAIN coatings was determined. The figure shows the resulting phenomenologic phase diagram.

We found a new route to increased hardness at high temperatures in metastable multilayer coatings. The figure shows the improved hardness at very high temperatures.
Plasma & Coatings Physics

STAFF
Ulf Helmersson, Professor
Nils Brenning, Guest Professor
Kostas Sarakinos, Associate Professor
Daniel Söderström, Assistant Professor
Iris Pilch, Post-doctor
Mattias Samuelsson, PhD-student
Montri Aiemparakit, PhD-student
Asim Aijaz, PhD-student
Daniel Magnfält, PhD-student
Viktor Elofsson, PhD-student
Bo Liu, PhD-student
Marta Saraiva, Visiting Scientist
Robert Boyd, Research Engineer
Sankara Pillay, R&D Project Manager
Mikael Amlé, Administrative Assistant

ASSOCIATE MEMBERS
Daniel Lundin, CEO at Ionautics AB
Peter Münger, Docent in the Theory & Modeling Division, IFM

INTRODUCTION
The Plasma & Coatings Physics group is a division at the Department of Physics, Chemistry and Biology (IFM), Linköping University, Sweden. Our overall goal is to contribute towards addressing challenges of contemporary materials science and technology through the synthesis of novel films and nanomaterials. To realize this goal, we employ innovative processes which allow for the generation of plasmas with unique properties as well as control of the material synthesis at the atomic level. Through a combination of advanced experimental and theoretical tools we seek to understand the process-plasma-material interactions and gain insight into the knowledge-based synthesis of functional films and nanomaterials.

SCIENTIFIC HIGHLIGHTS IN 2012
Nanoparticles: Synthesis & characterization
Our novel high power pulsed-plasma based method for synthesizing nanoparticles (particles with sizes in the range of a few to hundreds of nanometers) was developed further during 2012. The method allows for the synthesis of nanoparticles of a wide range of materials with a narrow size distribution. The past year, we have focused on the materials (silver and copper) and how the process parameters and the geometry of the experimental set-up affect the nanoparticle growth. It was found that the different geometries of the experimental set-up greatly affect e.g. the sizes of the nanoparticles. To get a fast response on the mass of the synthesized and collected nanoparticles when the process parameters are changed, research on using a quartz crystal microbalance (QCM) for this purpose was initiated. Preliminary results show that the QCM can be a valuable tool to determine “sweet spots” for the process (see Fig. 1).

A new compact vacuum system for the synthesis of nanoparticles was procured during the year. It will be devoted to the synthesis of oxide nanoparticles, e.g. copper and zirconium oxides, which will find applications in projects that are run in collaboration with other groups at the university.

Work on a computer simulation of the nanoparticle growth in a highly ionized plasma was initiated. The computer model will allow us to see how the plasma parameters will affect the collection efficiency of ionized material to the nanoparticles, and will help us to understand the fundamental processes we observe in the experiments. A manuscript is planned to be submitted during the first half of 2013.

Research on core-shell nanoparticles was continued with a major re-design of the synthesis chamber. We now have the opportunity to accurately sift ready-made particles through our coating zone. This allows us to study the coating of nanoparticles before we combine the processes to synthesize both the core and the shell in a continuous process.

During the year, two manuscripts were submitted to peer-reviewed journals.

Control of film nucleation and growth using ionized pulsed vapor fluxes
We have used pulsed, ionized fluxes generated by a HiPIMS discharge to deposit Ag films on SiO2 substrates. We have found that the time domain of the deposition flux (controlled by the pulsing frequency), the instantaneous vapor arrival rate and the energy of the film forming species (control by the pulse energy) enable one to tailor film nucleation and growth, manifested by the changes in the film thickness required for the completion of the film coalescence (Fig. 2).


Fig. 1. Deposited mass of nanoparticles as a function of pulse frequency for different peak currents. The pulse width was 30µs and the pressure 0.8 Torr.
Atomistic mechanisms for stress generation in physically vapor deposited films

We have studied the stress evolution in Mo films grown by HiPIMS. We have found that, depending on the energetic bombardment encountered by the growing film (controlled by the process conditions), films with intrinsic stresses ranging from highly compressive to slightly tensile are obtained. No correlation between the stress and the stress-free lattice parameter has been observed (Table I) indicating no changes in the concentration of intra-grain point defects. On the contrary, compressive stress generation is associated with increase of the film mass density (Table I). Based on these results, we have concluded that compressive stresses are generated via grain boundary densification through incorporation of film forming species. Atomistic mechanisms that lead to diffusion of film forming species into grain boundaries have been suggested.

Reference: D. Magnfält et al., “Atomistic mechanisms leading to insertion of adatoms into grain boundaries and compressive stress generation in physically vapor deposited film”, in final preparation.

Table I. Effect of deposition conditions (pw and PTp) on stress (σ), stress free lattice constant (a₀), and film mass density (ρm)

<table>
<thead>
<tr>
<th>pw (Pa)</th>
<th>PTp (kW)</th>
<th>σ (GPa)</th>
<th>a₀ (Å)</th>
<th>ρm (g/cm³)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.16</td>
<td>152</td>
<td>-3.0±0.4</td>
<td>3.152±0.003</td>
<td>10.29</td>
</tr>
<tr>
<td>0.4</td>
<td>66.4</td>
<td>-2.4±0.3</td>
<td>3.151±0.003</td>
<td>10.205</td>
</tr>
<tr>
<td>0.16</td>
<td>45.5</td>
<td>-2.3±0.2</td>
<td>3.151±0.002</td>
<td>10.11</td>
</tr>
<tr>
<td>0.4</td>
<td>28</td>
<td>-1.4±0.2</td>
<td>3.150±0.002</td>
<td>9.9</td>
</tr>
<tr>
<td>0.4</td>
<td>16</td>
<td>+0.2±0.2</td>
<td>3.150±0.003</td>
<td>9.82</td>
</tr>
<tr>
<td>0.4</td>
<td>4.5</td>
<td>+0.2±0.2</td>
<td>3.151±0.003</td>
<td>9.86</td>
</tr>
</tbody>
</table>

We have investigated the tilt of the columnar microstructure in Cu and Cr films deposited off-normally from highly ionized fluxes generated by a HiPIMS discharge. We have found that the film columns are positioned closer to the substrate normal as the ionization degree of the incident vapor increases (Fig. 3). This correlation between column tilting and degree of ionization is, however, valid only at certain kinetic conditions during growth (Cu but not Cr films at room temperature), indicating that the film morphology during the nucleation stage also affects the resulting column tilt (Fig. 3). A phenomenological model that explains, qualitatively, the column tilt accounting for atomic shadowing at different nucleation characteristics has been suggested.


Synthesis of carbon-based thin films using HiPIMS

We continued to explore the potential of HiPIMS for the synthesis of carbon based thin films in the year 2012. We developed a HiPIMS based process for the synthesis of hydrogenated amorphous carbon (a-C:H) thin films. The process is based on the hybrid arrangement of HiPIMS and DCMS, whereas the film synthesis is performed using a hydrocarbon precursor gas (acetylene) mixed with argon. We have found that the a-C:H thin films with low H content (about 10%) can be grown at about ten-fold higher deposition rate as compared to those deposited in pure argon ambient using an acetylene fraction of 5% in the gas mixture. The films, along with low H content, exhibit high hardness (more than 25 GPa) while the mass densities of the films in the order of 2.32 g/cm³ are obtained (Fig. 4).

HIPIMS – REACTIVE SPUTTERING

Discharge current behavior in reactive HiPIMS

In a more recent work, we investigated the behavior of the discharge current in reactive HiPIMS processes of metal-oxides (Ti-O and Al-O). The investigations were carried out by measuring the ionized contributions of the sputtering and reactive gas ions (Ar+ and O+) respectively, sputtered metal ions (Ti+ and Al+) as well as material-dependent properties (secondary electron emission yield and partial sputtering yield), to the discharge current. The ionized flux of the plasma species, Ar+, O+, Ti+ and Al+ was obtained by measuring the time-averaged and time-resolved ion energy distribution functions using ion mass spectrometry while the secondary electron emission and partial sputtering yields were obtained by performing TRIDYN simulations.

It was found that the observed increase in the discharge current in the oxide mode is due to the substantial contribution of O+ ions to the discharge current while the source of these O+ ions is the sputtering target rather than the gas phase.

Reference: M. Aiempanakit et al., “Understanding the discharge current behavior in reactive high power impulse magnetron sputtering of oxides”, submitted for publication.

SYNTHESIS OF WEAR-RESISTANT, ANTI-REFLECTIVE COATINGS USING HIPIMS

We have used HiPIMS to synthesize Al-Si-O wear-resistant antireflective coatings. Broad band anti-reflective multilayer coatings require the use of a low-index material at the top position. Normally SiO2 is used which exhibits sufficiently low refractive index (~1.5 at 550 nm) yet its low hardness (~10 GPa) hinders its application in abrasive environments. A strategy to circumnavigate these limitations is the synthesis of multicomponent materials that combine good mechanical and optical performance. We synthesize Al-Si-O films seeking to combine the low refractive index of SiO2 and the relatively high hardness of Al2O3. HiPIMS is used to enhance film properties, such as density and hardness. The work is performed in the framework of the EU project NoScratch (Grant agreement no 286697) in which our group is one of the RTD performers.

AWARDS 2012

- Asim Aijaz received the first Young Scholar Award at the International Conference on Diamond and Related Materials (ICDCM) 2012, Granada, Spain for his research on the synthesis of amorphous carbon thin films using HiPIMS.

INVITED LECTURES GIVEN DURING 2012

- U. Helmersson, *Opportunities using HiPIMS*, The 13th International Conference on Plasma Surface Engineering, Sept. 10-14, Garmisch-Partenkirchen, Germany, Tutorial presentation

SPIN-OFF COMPANIES GENERATED FROM THE GROUP:

- TiÅ AB, 2012
- Ionautics AB, 2010
- PlasmAdvance AB, 2007

ACADEMIC AND INDUSTRIAL COLLABORATION PARTNERS (OUTSIDE THE DEPARTMENT) IN ON-GOING PROJECTS OR JOINT PUBLICATIONS IN 2012:

- Prof. J.T. Gudmundsson and co-workers, Science Institute, University of Iceland.
- Drs. T. Kubart T. Nyberg and prof. S. Berg, Uppsala University.
- Prof. H. Kersten and co-workers, Kiel University, Germany.
- Prof. M.A. Raadu, KTH, Stockholm.
- Profs. J.E. Greene and I. Petrov, University of Illionois, USA.
- Dr. H. Ljungcrantz, Impact Coatings AB, Sweden.
- Prof. Ulf Jansson, Uppsala University, Sweden.
- Dr. E. Lewin, EMPA, Zürich, Switzerland.
- Prof. T. Minea and co-workers, Université Paris-Sud, France.
- Prof. J. M. Schneider, and co-workers, Materials Chemistry, RWTH Achen University, Germany.
- Dr. S. Kassavetis, Aristotle University of Thessaloniki, Greece.
- Prof. G. Abadías, Département Physique et Mécanique des Matériaux CNRS - Université de Poitiers - ENSMA, France.
- The group is also involved in industrial collaboration with companies in Sweden, Finland, France and Japan.
Semiconductor Materials

STAFF
Professors: Erik Janzén, Per Olof Holtz, Leif Johansson, Peder Bergman, Anne Henry, Nguyen Tien Son, Rozitsa Yakimova (emerita), Bo Monemar (emeritus).
Assistant professors: Jawad ul-Hassan, Gholamreza Yazdi.
Post docs: Philip Hens, Volodymyr Khranovskyy, Jianwu Sun, Somsakul Watcharinynanon.
PhD students: Supaluck Amloy, Charnseddine Boulhafs, Ian Booker, Ji-Tai Chen, Mihails Cubarofs, Daniel Dufåker, Martin Eriksson, Sadia Muniza Faraz, Andreas Gallström, Chih-Wei Hsu, Tomas Jemson, Valdas Jokubavicius, Xun Li, Louise Lilja, Anders Lundskog, Björn Lundqvist, Björn Magnusson, Daniel Nilsson, Susanna Stambach, Pontus Stenberg, Pitsiri Sukhaeva, Xuan Thang Trinh, Thien Duc Tran., Remigijus Vasiliauskas, Chao Xia, Mengyao Xie, Milan Yazdanfar.
Others: Annop Ektarawong, Tihomir Iakimov, Rickard Liljedahl.
Administrative/Technical staff: Eva Wibom, Sven Andersson, Roger Carmesten.

2. SUMMARY OF ACTIVITIES

The research activities in the Semiconductor Materials Division cover a broad spectrum, dominated by basic research. The projects are mainly funded by external agencies, partly with direct industry collaboration. There is a strong international cooperation within most research projects. The present research program can be divided into the following partly overlapping areas:

- Preparation and characterization of epitaxial films and bulk material of semiconductors with chemical vapor deposition (CVD), and sublimation techniques, with a strong emphasis on SiC and III-nitrides. The characterization includes surface and interface properties, structural properties, optical properties and transport properties.

- Investigation of properties of dopants and defects in a large variety of semiconductors, including structural as well as electronic properties. The latter covers bulk, surface and interface defects, with several techniques including laser spectroscopy and magnetic resonance.

- Preparations and investigation of the electronic properties of semiconductor quantum structures and nanostructures such as heterostructures, quantum wells, quantum wires and dots, and superlattices, with various spectroscopic techniques in several material systems.

- Studies of the electronic structure of III-nitride materials including defects and doping.

- Fabrication and characterization of graphene on SiC.

- Development of GaN and AlGaN/GaN HEMT structures for high-frequency power devices and Al-rich AlGaN heterostructures for laser diodes (LDs) and light emitting diodes (LEDs) in the UV (<400 nm) and deep UV (DUV, <300 nm) spectra regions.

- Growth and characterization isotope enriched SiC layers for improved spectroscopy, enhanced thermal conductivity, and for quantum computing studies.

Research activities in this division during 2012 have produced 73 papers published in high quality international journals, 26 conference proceedings papers with peer review and 3 review articles/book chapters. During the year, 15 invited talks were given by the staff at international conferences or symposia. The researchers of the division are well cited in international journals, the SCI citations of papers cited for the researchers in the division cover more than 22,000 ISI citations.

The highlights of the research work are presented at our website: http://www2.ifm.liu.se/semiconductor/. An updated list of publications 2012 can be searched in Linköping University (LiU) data base: http://liu.diva-portal.org/smash/searchlist.jsf?searchtype=postgraduate&organisation=semiconductor_materials&from=2012&until=2013

The turnover for research in our division was about 57.9 MSEK during the period 120101-121231, excluding equipment grants. The major part of this budget comes from external sources. The faculty support for research was about 8 MSEK for the year. External grants originate mainly from the Swedish Research Council (VR), the Knut and Alice Wallenberg Foundation (KAW), the Swedish Strategic Research Foundation (SSF), Swedish Energy Agency, European Defence Agency (EDA/FMV) and EU. In addition there is a strong support from and an intimate cooperation with several industries, mainly LG Innotek, Norstel AB and Aixtron AB, and with the Defense Research Institute FOI.

The Division was during 2012 engaged in several European research projects and Nordic project:

Manga and EuSiC are two large-scale joint multinational initiatives of leading system houses and research laboratories in Europe aiming at the development of independent and state-of-the-art capability in GaN HEMT technology. The goal of EuSiC is to develop high quality European GaN-Wafer on SiC substrates for space applications and to create an independent European supply chain for space technology.

NORLED – The N-Inner project with partners from Sweden, Denmark, Germany and Norway explores fluorescent silicon carbide for light emitting properties. A paper that describes the research was included in the Physica Scripta Highlights of 2012. This collection celebrates the most influential research published in the journal from the last 12 months.

LG-Innoteck – The project, which is sponsored by LG Innotek and the State of South Korea, strives to develop uniform epitaxial layers for power device material on 4” wafers using the chlorinating epitaxial process that has been studied here for several years. The first phase (three years) of the project has been concluded and the next phase is about to commence. During the coming phase the focus will be on reducing the density of structural defects that are harmful to the device performance and increase and control the lifetime of the material which is an essential part in the fabrication of bipolar devices.

A major part of the KAW project is devoted to isotope enriched SiC mainly for improved thermal conductivity. Isotope enriched SiC layers manifest a number of interesting properties useful for scientific and industrial applications. Among them is a very narrow linewidth in optical characterization which enables detailed measurements of defect centers. Another interesting phenomenon of the enriched layers is that they exhibit significantly higher thermal conductivity due to a reduced isotope scattering process in the material. We produced a number of isotope enriched epitaxial layers which we used to measure thermal conductivity on. The measurements told us that we indeed could see a substantial improvement in thermal conductivity yet we have not
yet been able to firmly establish the magnitude of the increase as compared to natural SiC. In light of the favorable outcome of these experiments we managed to secure a larger amount of enriched precursor gas to continue our experiments. A novel reactor which is specially designed to reduce contamination from foreign isotopes is being constructed.

The SSF project SiC—the Material for Energy-Saving Power Electronics started in 2012 and is focussed on determining, understanding and improving material related issues in SiC epitaxy and gate dielectrics, which today are the limiting factors for the SiC power device technology. The project includes: (i) Understanding and control of carrier lifetime limiting defects in SiC material and devices, (ii) Characterisation and identification of device-critical epitaxial defects, (iii) Investigation novel alternative gate dielectrics and novel fabrication techniques, (iv) Develop on-axis and/or low-off angle epitaxy for power device applications and (v) Develop Cl-based epitaxy for high growth rates.

Three PhD students (Remigijus Vasiliauskas, Anders Lundskog, Mengyao Xie) and four diploma works graduated in 2012. The Division is very active in teaching and has the responsibility for about 20 undergraduate and graduate courses at IFM.

3. HIGHLIGHTS
Chloride-based CVD growth of Silicon Carbide for Electronic Applications
A review paper on chloride-based SiC CVD was published in the highly renowned journal Chemical Reviews, highest ranked journal in the field of multidisciplinary chemistry (the 2011 impact factor is 4.0197). This is the first review of the field of chloride-based CVD for SiC. [H. Pedersen et al., Chemical Reviews 112, 2434 (2012)].

Low temperature CVD of boron-carbon films for neutron detectors
To enable CVD for the production of the novel neutron detectors based on the isotope 10B suggested by the European Spallation Source (ESS), novel low temperature CVD routes are needed. The neutron detectors will be based on aluminum, setting an upper temperature limit of 600°C and preventing the use of BCl3 as boron precursor. We have demonstrated the synthesis of thin, amorphous, boron-carbon films, with density and stoichiometry close to B4C, at ≤ 600°C by thermally activated CVD using the organoborane triethylboron, B(CaH3), (TEB) as single precursor. [H. Pedersen et al., Chem. Vap. Deposition 18, 221 (2012)]

A novel high-power pulse PECVD method
A novel plasma enhanced CVD (PECVD) technique has been developed in order to combine energetic particle bombardment and high plasma densities found in ionized PVD with the advantages from PECVD such as a high deposition rate and the capability to coat complex and porous surfaces. Ionized plasma is generated above the substrate by means of a hollow cathode discharge sustained in direct current (DC) mode, or in high-power pulsed (HiPP) mode using short pulses of a few tens of microsecond. [H. Pedersen et al., Surf. Coat. Technol. 206, 4562 (2012)]

Growth of semiconductor quality 3C-SiC
Cubic SiC was grown by a sublimation method. Bulk like material demonstrated that the 3C-SiC can reach similar quality like commercial hexagonal SiC. As an ultimate device property, in a 760 µm thick material the measured carrier lifetime is 8.2 µs, which is comparable with the best carrier lifetime in 4H-SiC layers. [J.W. Sun et al., Appl. Phys. Lett. 100, 252101 (2012)].

Shockley-Frank stacking faults in 6H-SiC
Shockley-Frank stacking faults (SFs) identified in 6H-SiC by a combination of low temperature photoluminescence and high resolution transmission electron microscopy. In the faulted area, stacking faults manifested as large photoluminescence emissions bands located in between the 6H-SiC signal (at ~ 2.99 eV) and the 3C-SiC bulk-like one (at ~ 2.39 eV). Each of the stacking fault related emission band had a four-fold structure coming from the TA, LA, TO and LO phonon modes of 3C-SiC [J. W. Sun et al., J. Appl. Phys. 113, 113527 (2012)].

Negative-U System of Carbon Vacancy in 4H-SiC
Using electron paramagnetic resonance (EPR), energy levels of the carbon vacancy (VC) in 4H-SiC and its negative-U properties have been determined. Combining EPR and deep-level transient spectroscopy, the two most common defects in as-grown 4H-SiC—the Z1/2 lifetime-limiting defect and the EH7 deep defect—have been identified to be related to the double acceptor (2-|o) and single donor (o|+) levels of VC, respectively. [N.T. Son et al., Phys. Rev. Lett. 109, 187603 (2012)].

The influence of substrate morphology on thickness uniformity and unintentional doping of epitaxial graphene on SiC
A major part of the research related to graphene on SiC prepared by high temperature sublimation has been focused on understanding the effect of the graphene surface morphology on its properties. Monolayer and bilayer graphene has been investigated. Effect of environment conditions has been studied as well. [J. Eriksson et al., Appl. Phys. Lett. 100, 241607 (2012); F. Giannazzo et al., Phys. Rev. B 86, 234422 (2012)].

Nucleation control of cubic silicon carbide on 6H-substrates
It has been demonstrated that when using 6H-SiC substrates 3C-SiC nucleates on a homoepitaxial layer grown prior to the cubic material. Ones nucleated 3C growth rate becomes higher than that of the 6H-SiC. Supersaturation has been calculated via thermal simulation in the growth cell and shown that the supersaturation non uniformities resulted in 6H-SiC inclusions. These findings were used to propose proper growth conditions of high quality bulk-like cubic SiC. Another project was to develop new substrates for optimized epitaxial graphene – cubic SiC [R. Vasiliauskas et al., Cryst. Growth and Design 12, 197 (2012)].
Detailed studies of Si intercalation-de-intercalation of graphene on 6H-SiC(0001)
The intercalation and de-intercalation mechanisms of Si deposited on monolayer graphene grown on SiC(0001) substrates and after subsequent annealing steps were investigated. After Si deposition on samples kept at room temperature, small Si droplets were observed on the surface, but no intercalation can be detected. Intercalation was revealed to occur at an elevated temperature of about 800 °C. The Si was found to migrate to the interface region via defects and domain boundaries. This observation may provide an answer to the problem of controlling homogeneous bi-/multilayer graphene growth on nearly perfect monolayer graphene samples prepared on SiC(0001). [C. Xia et al., Phys. Rev. B. 85, 045418 (2012)].

Changes in structural and electronic properties of graphene grown on 6H-SiC(0001) induced by Na deposition
The effects of Na deposited on monolayer graphene on SiC(001) were investigated. The experimental results show that Na prefers to adsorb on the graphene layer after deposition at room temperature. A fully Na intercalation at the graphene-SiC interface was obtained after heating at about 75 °C. Interestingly, the two bands show different locations of the Dirac point after heating and both exhibit linear dispersion in the vicinity of the point and not the hyperbolic dispersion observed for AB stacked bi-layer graphene. [S. Watcharinyanon et al., J. Appl. Phys. 111, 083711 (2012)].

Change in structural and electronic properties of graphene grown on 6H-SiC(0001)

Formation of nitride based pyramidal dots
InGaN quantum dots have been fabricated on top of hexagonal GaN pyramids by selective area growth using hot-wall metal organic chemical vapor deposition. To understand the growth mechanism of these InGaN QDs, correlated scanning transmission microscopy (STEM) and micro-photo-luminescence (µPL) measurements were performed. It is found that the InGaN QDs giving rise to sharp and well defined emission peaks in µPL spectrum is a consequence of a Stranski-Krastanov transition on a truncated area located at the apex of the hexagonal GaN pyramid (Fig. 4). [A. Lundskog et al., Nanotechnology 23, 305708 (2012)].

CVD growth of sp2-hybridized rhombohedral boron nitride.
(M. Chubarov, H. Pedersen, H. Höberg, A. Henry). The epitaxial growth of sp2-hybridized rhombohedral boron nitride (r-BN) using chemical vapour deposition has been investigated using ammonia and triethyl boron as precursors and sapphire as substrate. Hydrogen gas is necessary for the formation of r-BN, whereas its formation is considerably damped when using argon as the carrier gas. The presence of Si atoms in the process improves the crystalline quality of the growing film and contributes to the growth of high quality epitaxial r-BN instead of less ordered t-BN film. The incorporation efficiency is found rather low with an accumulation on the surface. [Cryst. Growth & Design 12, 3215 (2012) and Cryst. Eng. Comm. DOI: 10.1039/c2ce26423d].
Elastic constants, composition, and piezoelectric polarization in InxAl1-xN
We have reported for the first time a detailed study on the lattice parameters and stiffness constants of InxAl1-xN and discuss in detail their deviations from Vegard's rule, and effects on the determination of the alloy. We also reported for the first time the piezoelectric polarization behavior for InxAl1-xN with arbitrary surface orientations pseudomorphically grown on GaN and discuss the implications of the deviations from Vegard's rule in the lattice parameters and stiffness constants. The detailed discussions provide guidance to experimentalists on the appropriate approaches to estimate composition and piezoelectric polarization for InxAl1-xN with different compositions, surface orientations and degrees of strain. [M.-Y. Xie et al., Phys. Rev. B 86, 155310 (2012)].

\[ \text{Fig. 6. Piezoelectric polarization PPZ in InxAl1-xN grown pseudomorphically on GaN as a function of the inclination angle between the growth plane and the c-plane, } \theta, \text{ for different compositions, } x. \]

AIN and AlN alloys

Manga & EuSiC
Manga and EuSiC are two large-scale joint multinational initiatives of leading system houses and research laboratories in Europe aiming at the development of independent and state-of-the-art capability in GaN HEMT technology. Manga program is a continuation of the KORRIGAN program with dedication to build up a European supply chain of GaN HEMT technology. LiUs participation within Manga is material development with focus on interface properties between the SiC substrate and the nitride epilayer and to improve the thermal dissipation. The goal of EuSiC is to develop high quality European GaN-Wafer on SiC substrates for space applications and to create an independent European supply chain for space technology, Linköping University will grow HEMT structures on 3” wafers, which then will be processed at the European process house, United Monolithic Semiconductor, UMS in Germany.

THE SSF FUNDED NANO-N CONSORTIUM
Nitride based quantum dots and wires for optoelectronic applications
The NANO-N consortium is financed within the NANO-X program by SSF. The focus for NANO-N is towards nano structures made of the wide band gap semiconductors: GaN/AlN/InN based quantum wires and dots.

The organization of our NANO-N consortium
Consortium leader: Prof. Per Olof Holtz
Senior researchers: Prof. Erik Janzén, Prof. Jens Birch, and Prof Lars Ojamäe
Industry/institute mentors: Jan Andersson, Susan Savage, Teresita Kvarnström, Qin Wang, Acreo, Kista and Steven Savage, FOI, Linköping
Junior researchers: Fredrik Karlsson, Mattias Kula, Urban Forsberg, Maria Lundskog, Ching-Lien Hsiao, Reui-San Chen, Yen-Ting Chen
PhD students: Anders Lundskog, Chi-Wei Hsu, Supaluck Amloy, Justinas Palisaitas, Muhammad Junaid, Martin Eriksson

Within the NANO-N consortium, financed by SSF, nitride based quantum dots for optoelectronic applications are investigated. The focus is towards fabrication and optimization of photon emitting GaN/InGaN based quantum dots structures. Within the NANO-N project, the development of deterministic InGaN quantum dots (QDs) at the apices of GaN pyramids has been focused. For practical QDs device applications, the QDs must be positioned in a controllable manner in order to facilitate efficient device processing. Most InGaN quantum dots reported up to date, consist of QDs randomly distributed across a planar sample area. This is a consequence of the Stranski-Krastanov (SK) growth method, enabling self-assembly of the QDs. The growth of InGaN QDs at the apex of a hexagonal GaN pyramid is an elegant site controlled approach, which we have developed in our hot-wall MOCVD reactor. The reproducibility and performance of these site controlled pyramidal dots have now attained such a maturity that we can proceed with more detailed investigations of the optical and structural properties of the InGaN dots.

Nitride based pyramidal quantum dots
The GaN pyramids were produced by growing GaN on photo-lithographically-patterned substrates by means of selective area growth. On top of these pyramids, a thin InGaN/GaN quantum well and a GaN capping layer were grown. The growth process was tuned till the films had state of the art quality structural quality and comparable with the best InGaN materials presented in the literature. An InGaN QD is formed at the apex of the GaN pyramid due to the pronounced (tensile) strain at the apex. Tunable QD emission energy by varying the growth temperature of the InGaN layers is also demonstrated.

Ternary nitride based nano rods
Ternary Alx-xInxN nanorods have been produced by ultra-high-vacuum magnetron sputter epitaxy (MSE) by cosputtering high-purity Al and In targets under ultra-high-pure nitrogen atmosphere. The crystal structure of the nanorods is wurtzite without mixing zinc-blende phase. Although the Alx-xInxN nanorods have hexagonal cross-sections in geometry, the nanorods have phase separation and forms core-shell structure with higher In content in the core. Furthermore, self-assembled superlattices (SLs) in the rods were observed.
**Electron microscopy on nitride pyramidal quantum dots**
The superior spatial resolution and analytical capacity of the electron microscope has been employed to analytically investigate nitride quantum structures with a spatial resolution below 1 nm. Currently, we have investigated the pyramidal structures, in particular the truncated area of the pyramid on which is crucial for the formation of the quantum dots. By means of the world class electron microscopy in Linköping, these understandings will be employed to investigate in detail the localization, segregation and diffusion of quantum structures throughout the remaining period.

**Optical characterization of nitride quantum dots**
The formation of individual InGaN QDs grown on GaN micro-pyramid arrays is evidenced by observing single, sharp, excitonic emission lines of excitonic origin from various pyramids in the optical characterization by means of micro-photoluminescence (µ-PL). These µ-PL spectra demonstrate that our process gives a better controllability on the dimension and/or the composition of the dots compared to e.g. conventional SK dots.

**Surface and Semiconductor Physics**

**STAFF**

Professors: Göran Hansson, Head of Department
Roger Uhrberg, Head of Division
Wei-Xin Ni

Post-Docs: Jacek Osiecki

Ph.D. students: Hafiz Muhammad Sohail
Adm./Tech. staff: Kerstin Vestin, adm. asst., Karl-Olof Brolin, research eng., Chun-Xia Du, senior research eng., Ph. D.

**ACTIVITIES**
The research within the division of Surface and Semiconductor Physics includes the following fields. Firstly, basic studies are made of the electronic and atomic structure of semiconductor surfaces, either clean or with well-characterized overlayers. Foreign atoms on a surface may result in a large variation of ordered atomic structures, i.e., surface reconstructions. Physical properties like metallic or semiconducting surface conductance may depend on what reconstruction is formed. Various physical properties are studied using a range of different techniques. The most important one is photoelectron spectroscopy from which one can obtain a complete determination of the surface electronic structure. These studies are performed at the synchrotron radiation facility, MAX-lab in Lund, Sweden. Another important technique that we use is scanning tunneling microscopy (STM) that provides information about the atomic structure of the different surfaces. A variable temperature STM (Omicron) in our lab at IFM is the major instrument used for these studies. Over the period of several years we have also built up an experience in theoretical studies of various systems. We find the capability to do both experimental and theoretical studies quite important. It gives us the advantage that we can approach a problem from both the experimental and theoretical side to obtain a complete picture of the electronic and atomic structure.

Within this field, the division was supported by the Swedish Research Council (VR) as Roger Uhrberg has one research grant for studies of the atomic and electronic structure of semiconductor surfaces.

Secondly, there are studies, development and application of silicon-based molecular beam epitaxy (MBE), which is a crystal growth technique to produce advanced semiconductor structures.
for fundamental physics and device studies. We have also built up competence and process capability for the development of some device modules like SiGe-heterojunction bipolar transistors (HBT) for applications in optoelectronics and rf technologies.

Within this field, Wei-Xin Ni has recently gained one research grant from VR for studies of the silicon epitaxy on silicide templates for applications in extremely high frequency HBT technologies.

We are extensive users of the synchrotron radiation facility MAX-lab in Lund and over the years we have built up experimental equipment at two different beam lines. One of us, Uhrberg, is working actively with the angle resolved photoelectron spectroscopy (ARPES) beam line, which is one of the first seven to be built at MAX IV. The beam line, which will be located at the 1.5 GeV ring, has received a funding of 70.2 MSEK.

Courses

The division has during the year been responsible for the following undergraduate courses for students within the Engineering Programs and the International Masters Program on Material Science: TFYA18 Optoelectronics (Ni), TFYA25 Physics of Condensed Matter, part II (Uhrberg). The Ph. D. course Solid State Physics 1 was given by Uhrberg.

HiLIGHS

1) The structural and electronic properties of the two-dimensional Sn/Ag/Ge(111)3x3 surface alloy has been studied. This is a rare example of a system that forms a well ordered, one atomic layer thick, alloy. Experimental techniques like low energy electron diffraction (LEED), scanning tunneling microscopy (STM), and angle resolved photoelectron spectroscopy (ARPES) are complementary, and they combined provide both electronic and atomic structure information. Figures 1a and 1b present filled and empty state STM images of the same area of the 3x3 structure, respectively. The STM images are representations of the density of states within the energy range set by the tunneling voltage. The parallelograms drawn in Figs. 1a and 1b outline the unit cell that is nine times as large as that of the substrate. The filled state image is dominated by one protrusion while the empty state image shows two protrusions per unit cell. Each protrusion in the filled state images corresponds to several Sn and/or Ag atoms. The electronic structure that gives rise to the STM images can be studied in detail by ARPES. Fig. 1c shows the intriguing Fermi surface consisting of overlapping triangles at every K-point and a complex shape at G. The electronic bands that disperse across the Fermi level have a free electron like shape, with a high electron velocity. These steep bands, with almost linear dispersion, are clearly seen in Figs. 1d and 1e.

2) Following the earlier success in fabricating RF- and photonic-transistors using Si/SiGe-heterojunction structures made by molecular beam epitaxy (MBE) with improved performance, the group continues its effort in making Si-based epitaxial layer structures for advanced device applications. A growth technique has been recently developed, which enables the epitaxial growth of Si layers on some silicide templates.

Si-on-silicides or vice versa are highly interested for many device applications, in particular, SiGe-heterojunction bipolar transistors (HBTs) to operate at extremely high frequencies, e.g., with a fmax value beyond the 0.5 THz forecast of the International Technology Roadmap for Semiconductors (ITRS). One obstacle that blocks research was occurrence of the Si 3D growth due to a result of strong local distortion and a large bond-energy difference between Si and metal atoms, although the crystalline structures are similar with a very small lattice mismatch between Si and some silicides, e.g., CoSi2 (a0=5.364 Å compared to a0=5.430 Å for Si) and NiSi2 (a0=5.406 Å).

In our approach, the growth experiments were carried out on the patterned Si substrate, supplied by Uppsala University, with 6-nm thick Co-xNiSi2 strips of 1-10 µm in width. With an elaborate in situ surface cleaning process using a Si beam, and the substrate temperature modulation during growth to trade off the nucleation rate and dislocation propagation, defect-free Si layers with a thickness below 10 nm have been successfully grown on Co-xNiSi2 strips. The interface between Si and silicate was very flat and coherent, as evidenced by high-resolution transmission electron microscopy.

The group has also recently initiated some research activities aiming at developing the techniques that can produce an oxide layer on silicon-carbide (SiC) with improved interface properties and a high dielectric strength. By investigating the detailed chemical processes involved during the oxidation of SiC, we pro-
posed a new means to pre-treat the carbide surface, followed by the oxidation of a Si-based layer at low temperature. The initial results are positive, and we will continue the activities, in order to achieve a technology that would be used for manufacturing SiC-MOSFETs for power electronic applications.

ASSIGNMENTS
1. Scientific program committee of the 8th International Conference on Si Epitaxy and Heterostructures (ICSi-8, Fukuoka, Japan on June 2-7, 2013). Ni.

APPOINTMENTS
1. Prof. Wei-Xin Ni is currently an appointed associate editor of IEEE Transactions on Nanotechnology.

COLLABORATIONS
There is extensive collaboration with other groups at IFM for the characterization of MBE-grown structures, in particular the divisions of Semiconductor Materials and Thin Film Physics. External collaboration has been done with, e.g., groups at Johannes Kepler University (Prof. C. Pidgeon), Heriot-Watt University (Prof. C. Pidgeon), National Nano Device Labs in Taiwan (Drs. M.-N. Chang and J.-M. Shieh), Sichuan Institute of Solid State Circuits (Dr. K.-C. Li), Tsinghua University (Dr. D.-G. LiU). In projects involving synchrotron radiation we collaborate with Dr. K. Sakamoto, Chiba University, Japan.

MASTER THESIS WORK:
Yu-Wei Chiu: Novel method of SiC oxidation for the improvement of interface properties, June 2012.

Thin Film Physics

STAFF
Professors
Lars Hultman, Head of Division
Jens Birch, Deputy Head
Esteban Broitman, Guest Prof., Carnegie-Mellon
Michel Barsoum, Guest Prof., Drexel University
Joseph E. Greene, Guest Prof., University of Illinois
Anne Henry (from 2013)
Ivan Petrov, Guest Prof., University of Illinois

Associate Professors / Lecturers
Johanna Rosén, Senior Lecturer, Docent, Deputy Head
Valeriu Chirita, Senior Lecturer, Docent
Per Eklund, Senior Lecturer, Docent
Fredrik Eriksson, Senior Lecturer, Docent
Gueorgui Gueorguiev, Lecturer, Docent
Hans Högborg, Senior Lecturer, VR Researcher, Docent
Jens Jensen, Senior Lecturer, Docent
Martin Magnuson, Senior Lecturer, Docent
Per Persson, Senior Lecturer, VR Researcher, Docent
Galia Pozina, Senior Lecturer, Docent

Assistant Professors / Researchers
Björn Alling, Docent
Grzegorz Greczynski
Ching-Lien Hsiao
Carina Höglund, ESS AB
Jun Lu
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Per Sandström

Post Docs
Yen Ting James Chen, Natl Tsing Hua Univ Taiwan
Axel Flink, Impact Coatings AB
Andrej Furlan, Uppsala University and Linköping Univ.
Magnus Garbrecht, CAU Kiel and Technion Israel
Árni Sigurdur Ingason, University of Iceland
Petra Lunca Popa, Univ. Strasbourg, now U. Paris-Sud
Biplab Paul, IIT, Kharagpur
György Zoltán Radnoczi, MFA, Hungarian Acad. Sci.
Jeremy Leroy Schroeder, Purdue University
Mark Tucker, University of Sydney
Igor Zhirkov, Tomsk State University

PhD Students
Konstantinos Bakogiannis
Mikhail Chubarov (from 2013)
Martin Dahlqvist, Licentiate
Daniel Edström
Annop Ektarawong (from 2013)
David Engberg
Anders Eriksson, Licentiate
Hanna Fager, Licentiate
Amie Fallqvist
Mathias Forsberg
Cecilia Goyenola
Joseph Halim, also at Drexel University, USA
Mehulde Imam
Lars Johnson, PhD 2012, now at Sandvik AB
Linda Karlsson
Sit Kerdsongpanya, Licentiate
Ali Khatibi, Licentiate
Sergey Khromov, Licentiate
Hanna Kindlund
Chung-Chuan Lai
Ludvig Landålv (from 2013), Ind. PhD Stu-dent, Sandvik
Aurelija Mockute, Licentiate
Jumaid Muhammad, Licentiate
Marlene Mühlbacher (from 2013) also Leoben Univ.
Simon Olsson, Licentiate
Justinas Palisaitis, Licentiate
Andrej Petruhins
Davide Sangiovanni, Licentiate
Susann Schmidt, Licentiate
Steffen Sonderby, Licentiate, Ind. PhD Stu-dent, DTI
Lina Tengdelius
Olof Tengstrand, Licentiate
Christopher Tholander
Andreas Thore
Agne Zukausaite, Licentiate
Administrative and Technical Staff
Kirstin Kahl, Division Coordinator, AFM Coordinator
Camilla Karlsson, Division Coordinator, Linné Coord.
Inger Eriksson, Division Coordinator, retired 2012
Therese Dannetun, FunMat Vinnex Center Coordinator
Sven Andersson, 1st Research Engineer
Karl-Olof Brolin, Research Engineer, retired 2012
Thomas Lingefelt, 1st Research Engineer
Harri Savimäki, Research Engineer

AIMS AND VISION
We conduct application-inspired basic research on thin films to fundamentally understand the atomistic nature of materials properties and behavior and learn how to make materials perform better through new methods of synthesis and processing. Emphasis is put on the relationships between growth from the vapor phase, microstructure and properties of advanced functional materials. We thus extend the frontiers of materials and nanosciences to expand the scientific foundations for the development of materials. Our research concerns unsurpassed design of new multi-functional materials for engineering, electronics, and the life sciences. Results are explored in collaboration with industry and the properties of structures unique to thin films form the basis for new and improved materials and processes. We further seek novel phases and structures, as well as discovering materials phenomena.

RESEARCH PROGRAM
Our research concerns the materials science and nanotechnology of thin films. It is aimed at increasing the understanding of vapor phase deposition, ion-surface interactions, and reactions in advanced materials. Specifically, we probe into the nature of epilayers, textured thin films, and nanoscale materials. Model systems include transition metal nitrides, wide-band gap nitrides, multifunctional ceramics (MAX phases; e.g., Ti3SiC2, Ti2AlN), nanocomposites, superlattices, fullerene-like compounds, low dimensional phases, cluster-assembled materials, and multilayers. The core techniques operated and developed by the Thin Film Physics Division are:

- Magnetron Sputter Epitaxy
- HIPIMS, in particular hybrid techniques
- Cathodic Arc, incl pulsed filtered
- Electron Microscopy: Cs-corrected, FIB, CL
- X-ray Diffraction, incl. RSM
- Nanotribology
- Ab initio Calc., incl Synthetic Growth Concept
- Molecular dynamics simulations

Individual Excellence Grants
- ERC Advanced Grant (Hultman)
- ERC Starting Grant (Rosén)
- KAW-Scholar (Hultman)
- KAW Academy Fellow (Rosén)
- SSF Ingvar Carlsson Award (Eklund)
- Vinnova Winnmer: III-N nanostructures (Pozina)
- VR Break-Through Research Grant (Pozina)

Center-of-Excellence and Coordinated Grants
- Strategic Grant (SFO) in Materials Science, AFM
- SSF Synergy Grant, FunCase

UNDERGRADUATE COURSES OFFERED
TFYA21 Materials Science (Hultman)
TFYA50 CDIO – Computational Physics (Chirita)
TFYA53 Computational Physics (Chirita)
TFFM 40 Analytical Methods in Mtrl Sci. (Chirita)
TFYA43 Nanotechnology (Birch)
NFYA04 Nano Scientific Project (Rosén)
TFYA17 Advanced Project Appl. Phys. (Ekund)
TFFE1 Electr. Measurem. Systems (Sandström)
TFMT11 Measurement Technology (Sandström)
TFMT16 Computers in Measurem. Syst. (Sandström)
TSTE05 (IFM) Electr. & Meas. Tech. (Sandström)

GRADUATE COURSES OFFERED
Synchrotron Radiation (Magnusson)
Ion Beam Analysis of Condensed Matter (Jensen)
Fundamentals of Ceramics (Barsoum)
Nucleation and Growth (Greene, Birch, and Hultman)
Vacuum Science and Technology (Ekund)
Electron Microscopy (Persson)
X-ray Diffraction (Birch and Eriksson)

PHD TESSES IN 2012
Lars Johnson, Inside The Miscibility Gap: Nanostructuring and Phase Transformations in Hard Nitride Coatings
Muhammad Junaid, Magnetron Sputter Epitaxy of GaN Epilayers and Nanorods

/licence theses in 2012
Hanna Fager, Growth and Characterization of Amorphous TiAlSiN and HfAlSiN Thin Films
Sit Kerdsongpanya, Scandium Nitride Thin Films for Thermoelectrics
Sergey Khromov, The Effect of Mg Doping on Optical and Struc-
tural Properties of GaN
Aurelija Mockutė, Thin Film Synthesis and Characterization of New MAX Phase Alloys
Simon Olsson, Approximant Phases in Quasicrystalline AlCuFe Thin Films
Susann Schmidt, Carbon based Thin Films Prepared by HiPIMS and DCMS
Steffen Sønderby, Physical Vapor Deposition of Yttria-Stabilized Zirconia and Gadolinia-Doped Ceria Thin Films for Fuel Cell Applications
Olof Tengstrand, Me-Si-C (Me= Nb, Ti or Zr): Nanocomposite and Amorphous Thin Films
Agnė Žukauskaitė, Metastable YAlN and ScAlN thin films: growth and characterization

DIPLOMA THERSES IN 2012
Peter Carlsson, Combinatorial Thin Film Synthesis of Cr₂AlC; a Comparison of 2 Sputtering Methods
Kuo Chieh-Yi, Fabrication and Optical Properties of ZnO Nanocrystal/GaN Quantum Well Based Hybrid Structures

SPECIAL EVENTS IN 2012
• Johanna Rosén appointed KAW Fellow
• Per Eklund Senior Lecturer
• VR Break-Through Grant to Galia Pozina
• Dr Galia Pozina winner of the IVA Engineering Sciences "Mentor 4Research" Prize – a catalyst for Commercialization
• Lars Hultman winner of the Junior Faculty Prize 2012 at LiU for supporting the careers of junior researchers, thus creating a sustainable research environment
• Lars Hultman Editor-of-Chief and Per Eklund Editor for Rapid Communications of VACUUM.
• Ching-Lien Hsiao, Per Eklund, and Johanna Rosén received VR Young Researcher Grants
• VR Industry Graduate Student (Ludvig Landälv, Sandvik) Grant to Hultman, Alling and Eklund.
• 5-year SSF Synergy Grant: Functional Carbides and Advanced Surface Engineering FunCase.

SCIENTIFIC HIGHLIGHTS IN 2012
• We commissioned a Kratos Axis Ultra DLD XPS System (Porthos). It is a state-of-the-art spectrometer equipped with monochromatized Al Ka and Ag La photon sources and a low-energy, low-incidence angle ion sputter gun for high resolution depth profiling of thin films. Instrument is equipped with the imaging analyzer that is capable of producing chemical state images with <3 mm spatial resolution. An in-situ heating stage (1000 °C) is available.
• Together with researchers of ESS AB we presented a method to produce thin films of \( \text{a-B, C} \), with maximized detection efficiency, intended to be part of a new generation of large area neutron detectors.
  \[ \text{J. Appl. Phys. 111 (2012) 104908} \]
• We found by ab initio calculations and synthetic growth that fullerene-like sulfolcarbide (FL-CSx) is structured for 10-20 at.% S. Both quasi-planar networks and cage-like conformations form, but bond rotation and cross-linking have a minor role.
  \[ \text{J. Phys. Chem 116 (2012) 21124} \]
• Chromium carbide thin films were found to form amorphous nanocomposites with non-crystalline CrCx in an amorphous carbon matrix. Our soft X-ray absorption-emission study performed at MAX-IV Lab. shows additional peak structures exhibiting non-octahedral coordination and bonding.
  \[ \text{J. Phys. Cond. Mat. 24 (2012) 225004} \]
• The origin of the anisotropic Seebeck coefficient (thermoelectric effect) in nanolaminated crystals was traced to anisotropies in element-specific electronic states by using polarized angle-dependent X-ray spectroscopy. Our results explain why the average Seebeck coefficient of Ti₃SiC₂ in polycrystals is negligible over a wide temperature range.
  \[ \text{Phys. Rev. B 85 (2012) 195134} \]
• We employed a simplex-optimization procedure to predict that the hypothetical Nb2GeC MAX phase is stable, after which we discovered this Nb2GeC phase in theoretically guided thin film synthesis using magnetron sputtering. This is the first new 211 MAX phase to be discovered since the 1960s. Phys. Rev. Lett. 109 (2012) 035502.

• The structural perfection of fcc-ZnMgY single-grain quasicrystals was investigated using XRD and TEM in the Linköping aberration-corrected Titan3. Reciprocal space mapping analysis revealed a linear phason strain, which is a quasi-crystalline specific defect related to atomic rearrangements in the quasi-lattice. TEM revealed an unusually large phonon strain of up to 5% in film AlCuFeSi quasicrystal approximants.

• We used metastable NaCl-structure TiAlN as a model system to probe the effects of Al vs. Ti ion irradiation during film growth employing a hybrid approach combining high-power pulsed magnetron sputtering (HIPIMS) with dc magnetron sputtering. We showed that Al+ ion flux from HIPIMS target results in high-AlN content films with high hardness and low residual stress, unlike the growth assisted by Ti+/Ti2+ ions. Surf. Coat. Technol. 206 (2012) 4202

• We used VN as a model system to demonstrate, with experiment and DFT calculations, that refractory VMoN alloys exhibit not only enhanced hardness, but increased ductility. The hardness of newly synthesized V0.5Mo0.5N is ~25% above that of VN. While nanoindentated VN and TiN samples suffer from severe cracking typical of brittle ceramics, V0.5Mo0.5N films do not crack. Instead, they exhibit material pile-up around nanoindents, characteristic of plastic flow in ductile materials. In addition, the wear resistance of V0.5Mo0.5N is considerably higher than that of VN.

• CuO nano materials have interesting properties, depending on their nanostructures. Collaboration with Physical Electronics and Nanotechnology group in Norrköping. We have used HRTEM together with SAED studied the 3D complex nanostructure and first time found out a 3D interpenetrated architecture with (101) twin structure in β-shape nano CuO. Results are published on-line in MRLs.

• In collaboration with Uppsala Univ. and KTH, we have investigated solid-state-reactions to form nanoelectronic nickel silicides. Using the Linköping double-corrected Titan3 TEM we discovered a novel silicide with bcc structure, which is a metastable intermediate phase and play an important role for reduced-temperature formation of ultrathin epitaxial NiSi2 films.

• The distribution of an A element strongly influences the properties of Me1-xAx Zy, ternary materials, where Me is early transition metals, A is Al or Si and Z is C or N. We used our double-corrected Titan3 TEM combined with energy dispersive X-ray analysis to study the Si distribution in magnetron sputtered TiSiNy films grown on TiN-templated MgO(001), (110), and (111). Si segregation to form SiNz (z = i) tissue phases, which promotes formation of epitaxial TiN-enriched nanocolumns with {110} interfaces and {200} top facets.
TECHNOLOGY TRANSFER AND INTERACTIONS

- Granted Patent: Method for Producing a Neutron Detector Component: Carina Höglund (ESS), Jens Birch, Lars Hultman
- Patent issued: US 8,157,446 B2 “Cage for a roller bearing ...” L. Hultman with SKF AB
- Patent application: Coating of Substrates using HIPIMS: Lars Hultman, Grzegorz Greczynski with CemCon AG.
- Patent application: Graphene FETsensor, Ruth Pearce, Mike Andersson, Rositza Yakimova, Lars Hultman, Anita Lloyd Spetz
- ABB Corporate Research /Impact Coatings / SP for applications of MAX phases
- SECO Tools, Sandvik Coromant, Ion Bond, SKF, CemeCon: research on wear-resistant films and PVD processes
- N-works AB – a spin-off company started 2012 by Jens Birch and Lars Hultman
- Per Eklund and Sveriges unga akademi (SUA) published in DN-Debatt.

SCIENTIFIC BRANCH OF

Theory and Modeling

The program ‘Theory and Modeling (T&M)’ at the Department of Physics, Chemistry and Biology (IFM) includes Theoretical Physics, Computational Physics, Theoretical Biology, and Bioinformatics. The field of theory and modeling is presently in a very expansive phase. The reason is the profound and rapid development of computers, efficient algorithms, software, and immense databases that we experience today. It offers new and rich opportunities to solve in realistic ways many important problems. Moreover most challenging problems for modern science, the discovery of new and clean energy sources, understanding the structure of the Earth’s core, understanding mechanisms of protein function, solving the protein folding problem, and understanding the ecological consequences of global climate change require truly interdisciplinary efforts. Only a few years ago the complexity associated with shape, intricate boundary conditions, different length and time scales, immense amount of data, etc., simply made it prohibitive to tackle problems of this kind. Today we consider them with great success.

The general field of theory and modeling is also becoming increasingly important because it may supplement expensive and/or time consuming experiments and product developments with realistic simulations based on mathematical models, rapid access to large databases, etc. It may also replace hazardous, dangerous and/or very expensive experiments and even substitute inaccessible experiments. It is also important to point out that though the disciplines at T&M represent broad scientific fields, from physics to biology, they all rely on a common core of mathematical modeling, mathematical/numerical methods, and simulations. The computational problems usually deal with complex systems that require a wide range of scientific knowledge: problem formulation, mathematical modelling, numerical analysis, programming for parallel execution, hardware solutions, tools for analysis and visualization etc.

There are about fifty persons actively engaged in T&M. To organize common activities within T&M there is a steering committee, which includes Igor Abrikosov (theoretical physics and head of theory and modeling), Bo Ebenman (theoretical biology), Bengt Persson (bioinformatics), and Sven Stafström (computational physics). Lejla Kronbäck, Anna Sundin, Anna-Karin Stål and Malin Wahlberg acted as administrative assistants. Members of T&M carry out innovative research. In 2012 we published 82 papers in international journals with referee system. Our papers are well cited. We gave large number of invited talks at international conferences. Members of T&M are active in undergraduate and graduate teaching.

IFM is a motivating place for conducting theoretical programs, because it offers close contact with experimental activities and educational programs in engineering and science. Another important aspect is the access to the computational facilities and expertise at the National Supercomputer Center (NSC). In particular, our groups and NSC are actively involved in Swedish e-Science Research Centre (SeRC). We are actively participating in the Interdisciplinary Materials Science Laboratory for Advanced Functional Materials (AFM). Both, SeRC and AFM are supported by the Swedish Government. We are involved in Linnaeus Strong Research Environment supported by the Swedish Research Council, in Strategic Research Centres “Multiflows”, “Center of Organic Electronics (COE)”, and FUNCASE supported by the Swedish Foundation for Strategic Research. Also, we are part of FORMAS Strong Research Environment “Centre of Excellence for Farm Animal Welfare Research”, as well as projects “Isotopic Control for Ultimate Material Properties” and “Nanoparticles by Pulsed Plasma” supported by Knut and Alice Wallenbergs Foundation.

T&M represents a broad and interdisciplinary research program. To find out more about each other research, we organize annual group meetings. “Theory and Modeling Day”. In 2012 we met on December 19 (see photo) and discussed climate modeling. The conference program included a visit and presentations at SMHI (Norrköping) followed by presentations of T&M alumni, working at SMHI, Christian Asker, Mattias Jakobsson, and Nina Håkanson, as well as a presentation from NSC by Johan Raber.
Bioinformatics

**STAFF**

- Bengt Persson, professor
- Björn Wallner, senior lecturer
- Thabit Alabsi, Masters student
- Joel Hedlund, Ph. D., also at NSC
- Lejla Kronbäck, administrative assistant
- Malin Larsson, Ph. D., BILS expert
- Fredrik Lysholm, Ph. D. student
- Robert Pilstål, Ph. D. student
- Anna-Karin Stål, administrative assistant
- Malin Wahlberg, administrative assistant
- Linus Östberg, Ph. D. student

**RESEARCH**

**Characterisation of protein families**


**Membrane protein structure prediction**

We develop methods that can predict the structure of fairly complex membrane protein topologies from sequence information alone. We have also extended these methods to utilise limited structural information such chemical cross-crosslinks, metal-bridges or predicted interactions to improve these predictions further. Membrane proteins are a class of proteins with a severe gap between its occurrence in the genomes (30%) and the fraction of known protein structure (<1%). At the same time they are highly interesting since they are the gates to the cell and are involved in a wide variety of functions such as signal transduction, transport and cell-cell recognition. They are also the main targets for drugs on the market today. Structural knowledge for this important class of proteins is crucial to understand function and to be able to model the effect at the molecular level of small molecules and drugs.

![Figure 1: Structural prediction of two salt-bridges that promotes helical hairpin membrane insertion. In a recent collaborative effort with experimental groups in Spain, we used computational modelling to explain mutational data (cf. Figure 1).](image1)

**Prediction of protein domain interaction**

We are developing methods that utilize the massive amount of growing sequence data available to find subtle compensatory single point mutations in protein domain to predict interaction surfaces and exactly which residues that interact (cf. Figure 2). This information will improve both docking and structure prediction. The result for single domain proteins is fantastic, around 70% accuracy given enough sequence homologs (>1000 seq).

![Figure 2: Predicted residue contacts in the interface of a two domain protein highlighted in sticks, domain 1 in cyan and domain 2 in magenta.](image2)

**Protein model quality assessment**

With the rapid increase in computer power it is now easy to generate thousands of alternative models for a given protein sequence, using different methods and alternative alignments. This has transformed the field of protein structure prediction from predicting one single structure to selecting one structure for a large set of alternatives. We have pioneered in this field with both our consensus-based methods (http://pcons.net) and with our machine learning based model quality assessment programs, ProQ and ProQM. Our latest version of ProQ, ProQ2 was ranked no 1 in its class at CASP10, the biennial community-wide assessment of these methods.

**Structural calculations and predictions**

We use molecular modelling techniques to study molecular interactions and sequence variations in relation to structural changes. This methodology is applied to predict the effects of mutations in cancer-related proteins.

Facilitating analysis of massive amounts of sequencing data Bioinformatics methods and strategies have been developed for usage in large-scale metagenomics projects. These include an automated highly efficient BLAST search and result analysis pipeline, a novel alignment algorithm to produce more robust and accurate results with 454 data, and a new alignment tool HAXAT, allowing for on-the-fly correction of sequence read errors. The novel techniques have been used to analyse naso-
pharyngeal aspirates of children suffering from severe lower respiratory tract infections.

ELIXIR

ELIXIR, the European infrastructure for biological information, is now in its implementation phase. Bengt Persson is on the steering board, and BILS is establishing the Swedish node, which will start its activities in 2013.

BILS

The research infrastructure BILS – Bioinformatics Infrastructure for Life Sciences – has increased its activities during the year with over 250 projects nation-wide. BILS is coordinated from Linköping University, and Bengt Persson serves as director.

SeRC

IFM Bioinformatics is very active in the recently started Swedish e-Science Research Centre (SeRC), where Björn Wallner coordinates the bioinformatics community.

Teaching

During 2012, we have arranged courses in bioinformatics:
- at LiTH (TFTB29 and TFB14 autumn 2012)
- at HU in collaboration with IBK (spring 2012)

Popular science

Bengt Persson is on the organising committee of the annual research school at the Nobel manor Björkborn, Karlskoga, for 2nd/3rd year of Swedish high school students.

PhD students: Elham Mozafari, Jonas Sjöqvist, Cecilia Goyenola, Olle Falkløf, Thomas Fransson, Paulo V C Medeiros, Baswanth Oruganti, Riccardo Volpi

Adm. Assistants: Lejla Kronbäck, Anna-Karin Stål, Malin Wahlberg

GENERAL

In their work to describe electronic structure and electronic motions in molecular materials, the Computational Physics group employs a wide variety of methods including molecular mechanics and molecular dynamics for studies of structures and morphology, first principles electronic structure theory, response theory (for spectroscopic applications), DFT and TD-DFT, QM/MM methods, finite size scaling for studies of electron localization, the Landauer formalism, electron lattice dynamics and Monte Carlo methods for studies of charge transport. Most of the systems that we are studying are based on carbon but also silicon based systems, III-nitrides, etc are being modeled. The research cuts across a range of disciplines (molecular and supramolecular electronics, photonics, materials and polymer science, cluster-assembled compounds and low-dimensional phases, device physics, photochemistry and biochemistry) with many applications in the fields of nanotechnology, optoelectronics, and organic electronics.

The Computational Physics group gives a large number of courses on graduate as well as under-graduate levels: Classical Mechanics (undergraduate, MB), Quantum Mechanics (undergraduate, MB), Computational Quantum Chemistry (graduate, PN, ML, BD), Potential Energy Surfaces and Dynamics (NGSSC school, graduate, ML). Two diploma students have been working in the group during the year.

Patrick Norman was appointed director of the National Supercomputer Centre, NSC, at Linköping University.

The group organized the 2012 annual meeting of Svensk Teoretisk Kemi (STK), August 23-24, 2012.

HIGHLIGHTS


COLLABORATIONS WITHIN LIU

- Center in Nanoscience and Nanotechnology (CeNano)
- Center of Organic Electronics (COE)
- Thin-Film Physics, IFM
- Surface Physics and Chemistry, IFM
- Biomolecular and Organic Electronics, IFM
- Semiconductor Materials, IFM
- Organic Electronics, ITN

Computational Physics

STAFF
Professors: Patrick Norman, Sven Stafström (head of division)
Associate professors: Magnus Boman, Gueorgui Gueorguiev, Bo Durbeej, Mathieu Linares
Postdocs: Jonas Björk, Joanna Kauczor, Chang-Feng Fang
EXTERNAL ACTIVITIES AND NETWORKS

- Secretary general, Swedish Science Research Council, secretary general (SS)
- Board member, Nordforsk (SS)
- Director, NSC (PN)
- Unimolecular Electronics Center, Uppsala University
- Swedish Research Establishment
- Co-authoring the DALTON and DIRAC programs (PN)

INDIVIDUAL EXTERNAL COLLABORATIONS

- H. Ågren (KTH, Stockholm)
- T. Saue (Toulouse, France)
- F. Hanke (Liverpool, UK)
- K. Ruud (Tromsø, Norway)
- N. Avarvari (Angers, France)
- D. Beljonne (Mons, Belgium)
- R. Rivelino, F. Brito (Federal University of Bahia, Salvador, Brazil)
- J. Hellwell (Manchester, UK)
- Fernando Nogueira (Coimbra, Portugal)
- J. Barth (Technische Universität München, Germany)

External funding

External funding is absolutely essential for the activities in the computational physics group. We are grateful for support from a number of sources including the Swedish Research Council (VR), European Commission, Foundation for Strategic Research (SSF), Swedish Defence (FMV), Carl Trygger Foundation, Olle Engkvist Foundation and International Science Programme (ISP). In particular, Patrick Norman is “rådsforskare” at VR. Bo Durbeej has a VR grant for young researchers, Mathieu Linares is supported by the Swedish e-Science Research Centre (SERC) and Gueorgui Gueorguiev has a Swedish Foundation for International Cooperation in Research and Higher Education (STINT) project for bilateral collaboration with the Federal University of Bahia in Brazil. High performance computing resources were provided by the Swedish National Infrastructure for Computing (SNIC) and the National Supercomputer Centre, NSC, at Linköping University.

Theoretical Biology

STAFF

Professors: Bo Ebenman (head of division), Uno Wennergren
Associate professors: Peter Münger, Tomas Jonsson (guest lecturer)
Postdocs: Anna Eklöf, Tom Lindström
PhD students: Sofia Berg, Peter Brommesson, Alva Curtsdotter, David Gilljam, Sara Gudmundson, Nina Håkansson, Linda Kaneryd, Jenny Lennartsson, Malin Setzer, Stefan Sellman, Torbjörn Säterberg
Administrative assistant: Anna Sundin

GENERAL

There are two research labs in the division of Theoretical Biology: Population and Community Ecology lab (PACE lab) headed by Professor Bo Ebenman and Spatiotemporal Biology lab (SPABIO lab) headed by Professor Uno Wennergren. Present research projects include:

- The response of ecosystems to species loss: using community viability analysis to quantify the risk and extent of extinction cascades (Bo Ebenman PI)
- Using sensitivity analysis to identify keystone species and keystone links in ecosystems (Bo Ebenman PI)
- The robustness of ecosystems to an increasingly variable world: effect of climate change on the structure and functioning of ecosystems (Bo Ebenman PI)
- The response of metacommunities to habitat and species loss: the role of local and regional processes (Bo Ebenman PI)
- Ecologically effective population sizes (Bo Ebenman PI)
- Population growth in heterogeneous landscapes: crop management strategies for effective biological control of pests (Uno Wennergren PI)
- Reducing the risk of spread of diseases (Uno Wennergren PI)
- Long term strategies for preserving species in a dynamic landscape (Uno Wennergren PI)
- Analysis and optimization of animal transport: logistics and animal welfare (Uno Wennergren PI)

Members of the group are involved in several courses at graduate as well as undergraduate levels including courses in ecology, population ecology – theories and applications, mathematical models in chemistry and biology, and conservation biology.

EXTERNAL ACTIVITIES AND NETWORKS

Participation in:

The ESF Research Networking Programme SIZEMIC (Body-size and ecosystem dynamics: integrating pure and applied approaches from aquatic and terrestrial ecology to support an ecosystem approach). The programme is funded by the Swedish Research Council (VR) and several other national research councils in Europe. Bo Ebenman is a member of the steering committee of the programme. Sofia Berg, Alva Curtsdotter, David Gilljam and Anna Eklöf (presently a post doc at the University of Chicago) are active in two of the working groups organized by the network.

Mathematics in the Living Environment (MILE). Erasmus/Socrates collaboration with York University.

EXTERNAL FUNDING

PACE Lab – Prof. Richard Law (York University, UK), Prof. Owen Petchey (University of Zürich, Switzerland), Dr. Guy Woodward (Queen Mary University of London, UK), Prof. Mark Emmerson (University of Cork, Ireland), Prof. Ulrich Brose (Darmstadt Technical University, Germany) and Dr. Tomas Jonsson (Skövde University, Sweden).

SPABIO Lab - Prof. Mikael Rönnquist (Bergen University), Dr. Annie Jonsson (Skövde University), Prof. Bo Algner (SLU), Prof Colleen Webb (Colorado State University), Dr Michael Tildesley (Warwick University) and Docent Susanna Sternberg Iwerin (SLU).

EXTERNAL COLLABORATIONS

PACE Lab – Prof. Richard Law (York University, UK), Prof. Owen Petchey (University of Zürich, Switzerland), Dr. Guy Woodward (Queen Mary University of London, UK), Prof. Mark Emmerson (University of Cork, Ireland), Prof. Ulrich Brose (Darmstadt Technical University, Germany) and Dr. Tomas Jonsson (Skövde University, Sweden).

SPABIO Lab - Prof. Mikael Rönnquist (Bergen University), Dr. Annie Jonsson (Skövde University), Prof. Bo Algner (SLU), Prof Colleen Webb (Colorado State University), Dr Michael Tildesley (Warwick University) and Docent Susanna Sternberg Iwerin (SLU).

Mathematics in the Living Environment (MILE). Erasmus/Socrates collaboration with York University.
Theoretical Physics

STAFF
Professors: Igor Abrikosov (Head of T&M), Karl-Fredrik Berggren, Magnus Johansson, Bo Sernelius, Sergei Simak, Irina Yakimenko
Associate Professors: Peter Münger
Assistant Professors: Rickard Armiento, Weine Olovsson, Leonid Pourovskii, Ferenc Tasnádi
Postdoctoral fellows: Marcus Ekholm, Qingguo Feng, Ole Hellman, Peter Steneteg
PhD students: Viktor Ivady, Peter Jason, Hans Lind, Alexander Lindmaa, Igor Mosyagin, Olga Vekilova, Fei Wang

Administrative assistants: Lejla Kronbäck, Anna-Karin Stål, Malin Wahlberg
Masters students: Lasse Hultberg
Bachelor students: Gustaf Lundberg, Jesper Norell, Joakim Andersson, Felix Faber, Patrik Harrýsson
Project student: Johan Bergman
Visiting researchers: Prof. Lennart Stenflo, Sweden, Dr. Mathias Boström, Sweden, Dr. Alena Ponomareva, Moscow, Russia, Dr. Maxim Belov, Moscow, Russia, PhD student Anton Nikonov, Tomsk, Russia, PhD student Andrey Lugovskoj, Moscow, Russia, PhD student Pavel Korotaev, Moscow, Russia, PhD student Katarina Kirr, Kharkiv, Ukraine

APPOINTMENTS IN 2012
Sergei Simak was appointed professor of Theoretical Physics at Linköping University.
Magnus Johansson was appointed Director of Studies in Physics.
Rickard Armiento was appointed Assistant Professor.
Marcus Ekholm was appointed Postdoctoral Fellow.
Qingguo Feng was appointed Postdoctoral Fellow.
Ole Hellman was appointed Postdoctoral Fellow.
Peter Steneteg was appointed Postdoctoral Fellow.

GENERAL
The research in theoretical physics is focused on condensed matter physics/theoretical materials science, nanoscience, electromagnetic modeling, and non-linear physics. Typical projects are:
- Theoretical study of materials with fast ionic conductivity for energy applications (S. Simak, O. Hellman).
- Physics of strongly correlated materials (L. Pourovskii, M. Ekholm, Q. Feng, V. Ivady, I. Abrikosov).
- Theoretical spectroscopy (W. Olovsson).
- Materials modeling and high throughput energy material design (R. Armiento, A. Lindmaa, J. Bergman).
- Nanophysics, ultrasmall semiconductor structures and devices in the quantum regime, quantum information, transport, quantum and classical waves in cavities and constrictions with oscillating boundaries (I. I. Yakimenko, K.-F. Berggren).
- Nonlinear effects on energy transport in periodic and aperiodic spatially modulated systems (M. Johansson, P. Jason).
- Studies of dispersion forces in nanoscience, of the fundamental nature of the Casimir force and its temperature dependence (B. E. Sernelius and M. Boström).
- Gravitation as a Casimir interaction (B. E. Sernelius).
- Luminescence in ZnO nanorods, nanotubes and nanoparticles (B. E. Sernelius).

We participate in leading national research programs. In particular, we are actively involved in a new Swedish e-Science Research Centre and in the Interdisciplinary Materials Science Laboratory for Advanced Functional Materials, both supported by the Swedish Government. Igor Abrikosov is leading the Network for excellent research “Materials Science for New Energy Technology”. We are part of the Strategic Research Centers “Mutiﬁlms” and “FUNCASE”, both supported by the Swedish Foundation for Strategic Research. We, together with Computational Physics Group, build the node “Materials Modeling” within the Linköping Linnaeus Initiative for Novel Functional Materials, supported by the Swedish Research Council. Also, we participate in projects “Isotopic Control for Ultimate Material Properties” and “Nanoparticles by Pulsed Plasma” supported by Knut and Alice Wallenberg’s Foundation. At the European level, we were actively involved in European Network Psi-k, where Prof. Abrikosov is a spokesperson for Working Group “Alloy Theory”.

The theory group gives a large number of courses on graduate as well as undergraduate levels. The teaching has a wide range of courses, including analytical mechanics, quantum theory, relativistic quantum mechanics, condensed matter physics, many-body physics, statistical mechanics, quantum information and computing, elementary particle physics, cosmology, chaos and nonlinear phenomena. Peter Münger represents Linköping University in the ERASMUS Academic Network: Stakeholders Tune European Physics Studies - Two (STEPS TWO). It is a collaboration between more than 70 European Universities Physics Departments with the aim to investigate and improve various aspects of physics education.

PHD EXAMINATIONS
Marcus Ekholm, “Theoretical description of complex magnetism in transition metals and their alloys“, Dissertation No. 1452
Olle Hellman, “Thermal properties of materials from first principles“, Dissertation No. 1453
Peter Steneteg, “Development of molecular dynamics methodology for simulations of hard materials“, Dissertation No. 1454

2012 HIGHLIGHTS
Iron is the most abundant element on our planet. It is one of the most important technological materials and, at the same time, one of the most challenging elements for the modern
theory. As a consequence, the study of iron and iron-based alloys has been a focus of experimental and computational research over the past decades. While the structural properties of iron and iron-nickel alloys at pressures below 100 GPa are well established, their electronic and magnetic properties are still debated. Our state-of-the-art ab initio calculations of the Fermi surface of Fe within the dynamical mean-field theory (DMFT) reveal a change of its topology, the so-called electronic topological transition (ETT) at pressures of about 30–40 GPa (see the figure). The ETT manifests itself through anomalous behavior of the Debye sound velocity, \( c/a \) lattice parameter ratio and Mössbauer center shift observed by our experimental colleagues. The ETT is absent in one-electron calculations (see the figure) and represents a clear evidence of the importance of correlation effects in Fe at high pressure.


We analyze the occurrence of local magnetization and the effects of electron localization in different models of quantum point contacts (QPCs) using spin-relaxed density functional theory (DFT/LSDA) by means of numerical simulations. In the case of soft confinement potentials the degree of localization is weak and we therefore observe only traces of partial electron localization in the middle of the QPC. In the pinch-off regime there is, however, distinct accumulation at the QPC edges. At the other end, strong confinement potential, low-electron density in the leads and top or implant gates favor electron localization. In such cases one may create a variety of electron configurations from a single localized electron to more complex structures with multiple rows and Wigner lattices.

We first demonstrated how two-dimensional sheets are incorporated in the formalism for planar structures. Then we derived the interaction in the geometry of two freestanding graphene sheets and of one graphene sheet above a substrate. Numerical results were produced for the fully retarded interaction at \( T = 0 \) K and at room temperature for undoped and doped graphene. Additional results were given both for a gold substrate and for an ideal metal substrate. We found that for two freestanding undoped graphene sheets the retardation effects are negligible. The same holds for an undoped graphene sheet above a gold substrate. This behavior is very unusual and is the result of the particular band structure of graphene. However, for doped graphene sheets, two freestanding or one freestanding above a gold substrate, the retardation effects are bound to be important at large enough separations. However, at \( T = 300 \) K the retardation effects again go away.

The attractive retarded interaction energy as a function of separation, \( d \), at room temperature between (a) two undoped graphene sheets and (b) two doped graphene sheets. The separate contributions from TM and TE modes are shown. The interaction energy between two ideal metal half spaces is also shown as a reference result.


The increasing precision and tunability of ultracold atoms in optical lattices has greatly increased the interest for quantum lattice models, such as the Bose-Hubbard model. Ordinarily only interactions between bosonic atoms located on the same site are included, but extending the model with effects from longer-range interactions such as pair-correlated hopping between nearest neighbours may lead to new physical effects. We showed that this extended Bose-Hubbard model has exact one-site “Quantum Lattice Compactons”, being eigenstates with complete localization of all particles at one site. These appear at parameter values where the one-particle tunneling is exactly canceled by nonlocal pair correlations, and correspond in the limit of infinite particle number to exact compact solutions (“discrete compactons”) of a classical lattice model. Classical compactons existing at other parameter values, as well as exact multisite compactons, generically get delocalized by quantum effects, but strong localization appears asymptotically for increasing particle number. Compactons are interesting for applications due to their tail-less nature, prohibiting mutual interactions unless being in direct contact.

![Projection of the highest eigenstate on the single-site localized basis state as function of one-particle (Q2/N) and pair-correlated (Q2) hopping parameters, for (a) 16 and (b) 26 particles in a 4-site extended Bose-Hubbard model. The compacton appears as a white stripe.](image)
External activities and networks

- Swedish Physical Society (K-F Berggren, chairman, also Swedish delegate to European Physical Society Council); legally responsible for “Fysikaktuellt”.
- I. Abrikosov was a co-organizer of International Symposium and Workshop on Correlated Electrons and Materials Properties of Compounds and Alloys, Porto Heli, Greece.
- I. Abrikosov and S. Simak were co-organizer of International conference “Electronic structure theory for materials Modeling: from early days to current success”, Stockholm, Sweden.
- K-F Berggren was co-organizer of Nordita Workshop Spin2012: “Spin-Related Phenomena in Mesoscopic Transport”. Participation in:
  - Ψ Network.
  - NordForsk Network: Nanospintronics – Theory and Simulations (coordinator C. Canali, Linnaeus University of Kalmar, Sweden); I. Yakimenko node coordinator Linköping.
- Peter Münger participates in “The ‘Stakeholders Tune European Physics Studies - Two’ (STEPS TWO) initiative by the ‘European Physics Education Network’ (EUPEN) within the ERASMUS programme (http://www.stepstwo.eu/).

Individual external collaborations

- Igor Abrikosov and Prof. Michel Barsoum (Drexel University, USA), Prof. L. Dubrovinsky (Universität Bayreuth, Germany), Prof. M. I. Katsnelson (University of Nijmegen, The Netherlands), Prof. Yu. Kh Vekilov (Moscow Institute of Steel and Alloys, Russia), Prof. J M Schneider (Aachen University, Germany), Prof. J. Neugebauer (Max-Planck-Institut für Eisenforschung, Germany).
- Igor Abrikosov, Viktor Ivady, Rickard Armiento and Dr. Adam Gali (Hungarian Academy of Sciences).
- Bo Sernelius and Prof. G. D. Mahan (Penn State University, USA), Prof. Antonio Ferreira da Silva (Salvador de Bahia, Brazil), Prof. Barry Ninhin (Australian National University, Australia), Prof. Chris Binns (University of Leicester, England), Dr. Mike Ward, University of Birmingham, Birmingham, UK, and Dr. Astrid Lambrecht, École Normale Supérieure, Paris, France.
- Magnus Johansson with Dr. R. A. Vicencio (Universidad de Chile, Santiago), K. Kirr (National Academy of Sciences of Ukraine, Kharkiv), Dr. S. Derevyanko and Dr. Y. Prylepskyi (Aston University, UK), Dr. A.V. Yulin (Universidade de Lisboa, Portugal).
- Sergei Simak and Prof. O.M. Krasilnikov, Prof. Yu.Kh. Vekilov at NUST “MISIS”, Russia, Prof. N.V. Skorodumova at KTH
- Leonid Pourouvski and Marcus Ekholm with Prof. Antoine Georges, École Polytechnique, Paris, France
- K.-F. Berggren and I. Yakimenko with Prof. Sir M. Pepper (Cavendish Laboratory, Cambridge, UK and London Centre for Nanotechnology, UCL and with Prof. J. Bird (University of Buffalo, USA).
- Research Policy Institute, Lund University/Dept for Philosophy, Linguistics and Theory of Science, Gothenburg University (Olof Hallonsten/K-F Berggren)
- Peter Münger, collaboration with Anna Eklöf, University of Chicago, USA, the group of Tomas Jonsson at Högskolan i Skövde and Céline Hauzy at Universite Pierre & Marie Curie, Paris, France on “Dynamics in food webs - local and regional processes”.
- Weine Olovsson with the group of Prof. Claudia Draxl at Humboldt Universität zu Berlin (previously at Leoben University), the group of Prof. Isao Tanaka at Kyoto University, Japan, and Dr. Venkata Rama Rao Medicherla, Siksha ‘O’ Anusandhan University, Bhubaneswar, India
- Rickard Arniento and Ann E. Mattsson (Sandia National Laboratories, USA), Stephan Kümmel (University of Bayreuth, Germany), Predag Lažić (Rudjer Boskovic Institute, Croatia), Marco Fornari (Central Michigan University, USA), Boris Kozinsky (Robert Bosch LLC, USA).
- Olle Hellman and Prof. D. Broido, Boston College, USA

External visits

- Marcus Ekholm spent a total of one month at the École Polytechnique in Paris, France, with a support from the PHC Dahlén grant.
- Olle Hellman visited Boston College, USA, to initiate collaboration on thermal conductivity simulations.
- Viktor Ivady had a long-term visit to Hungarian Academy of Sciences.
- Igor Abrikosov visited Tomsk State University, Russia.
- Leonid Pourouvski has shared employment between IFM and École Polytechnique, Paris, France.
- Sergei Simak visited NUST “MISIS”, Russia.
- Magnus Johansson visited Universidad de Chile, Santiago.
- Weine Olovsson visited Kyoto University, University of Tokyo and Waseda University, Japan.

Popularization of science

- Start page of our group web site http://www.ifm.liu.se/theo-mod/theophys/ is used to present highlights of our recent research for the general public.
- Igor Abrikosov was interviewed for newspaper Dagens Industri enclosure “Forskning i Framkant” (November issue).
- Fysikaktuellt (K.-F. Berggren).
- “Parametric instabilities and pattern formation” Ohlin Laboratories, Uppsala (K Ohlin/K-F Berggren)
- Presentation of the Nobel Prize in Physics 2012 (I. Yakimenko for IFM and Y-program students).
- Magnus Johansson gave a talk “Quasi crystals and accelerating universe - infinities in the 2012 Nobel prizes” at the interdisciplinary symposium “A Day on Infinity” arranged by the department of Philosophy, LiU, 23 March 2012.
AFM

The Swedish Government Strategic Research Area (SFO-MatLiU) in Materials Science; International Interdisciplinary Materials Science Laboratory for Advances Functional Materials

**Director:** Prof. Lars Hultman  
**Deputy Director:** Magnus Berggren (ITN)

AFM encompasses 240 researchers from the departments IFM, ITN and IEI, and a partner ACREO, organized into interacting collaborating teams.

**MANAGEMENT BOARD:**
- Lars Hultman (Chair)  
- Magnus Berggren (Vice Chair)  
- Igor Abrikosov  
- Erik Janzén  
- Kajsa Uvdal  
- Hans Högberg (Research Manager)  
- Kirstin Kahl (Administrator)

AFM is in operation since 2010. It contributes at the highest level to the creation of knowledge. Materials science is a top research priority at Linköping University and strongly supported by industry and institutes. It is extremely productive as judged by both academic and societal metrics.

We envision that science is focused on the atomic/molecular-scale design of new materials will provide solutions to broadly-based societal issues, including jobs, health, energy, environment, and sustainability.

**OUR MISSION IS TO:**
1. Build a Coordinated Excellent Research Environment that integrates theory, simulations, and experiments  
2. Target and recruit internationally leading researchers in complementary fields  
3. Promoting tenure-track positions and career paths for young (star) researchers  
4. Investigate and open new and creative research fronts with commensurate industrial opportunities  
5. Create novel high-performance soft, hard, and hybrid smart materials  
6. Explore new concepts in synthesis, processing, analysis, and computer based modeling  
7. Provide for state-of-the-art laboratory settings. Invest in equipment with relevance for Sweden's infrastructure in synchrotron work, microelectronics processing, neutron facilities, supercomputing, and electron microscopy  
8. Link research to LiU’s large undergraduate, international master, and graduate programs and doctoral programs  
9. Expand core R&D capabilities by enlarging and protecting the IPR base of Swedish companies in key industrial sectors and foster new grass root spin-off companies  
10. Facilitate the introduction of novel smart materials, with specifically designed properties, into production by Swedish industry

**INDUSTRY REFERENCE PANEL:**
- Hans Hentzell, PhD, CEO Swedish ICT Research AB and Acreo AB
- Peter Isberg, PhD, Adjunct Professor (LIU), Technical Manager, Machines and Automation Products, ABB AB  
- Dr. Ingrid Reineck, PhD, Manager, Sandvik Tooling AB  
- Hans Sjöström, PhD, Docent, General Manager, SKF Nova  
- Jan-Eric Sundgren, PhD, Senior Vice President Public and Environmental Affairs, AB VOLVO

The charge to the industry Reference Panel is to provide benchmarking and a robust critique of the AFM’s performance in terms of technological transfer, problem-oriented research, industry collaboration, IPR policy and performance, statistics on spin-off companies and researchers places in industry.

**AGORA MATERIAE – THE MATERIALS SCIENCE GRADUATE SCHOOL**

Agora Materiae is our new graduate school with a multidisciplinary direction within Material Physics. It involves about 20 research groups/areas at IFM, IE, ITN, with an interest in hard and soft materials.

**Agora Materiae is managed by:**
- Per Olof Holtz (Head)  
- Stefan Klintström (Mentor)  
- Kirstin Kahl (Administrator)

**Agora Materiae Student Council:**
- Roger Magnusson, IFM, 2012  
- Jonas Bergqvist, IFM, Spring 2012  
- Linda Karlsson, IFM, Spring 2012  
- Martin Eriksson, IFM, 2012  
- Thomas Fransson, IFM, 2012  
- Zia Ullah Khan, ITN, start Fall 2012  
- Mattias Calmungere, IEI, start Fall 2012

**AFM HIGHLIGHTS 2012**

We started the Graduate School AGORA MATERIAE in Materials Science (see separate section for more information).

Researchers of the AFM environment is taking part in the Graphene Flagship.

One paper accepted in *Nature Nanotechnology* on the Magnetic quantum ratchet effect in graphene.

We published in *Science* the first generation of biopolymer based polymer electrodes of relevance for energy storage in supercapacitors and possibly in secondary batteries.

The first reported complementary and integrated chemical circuits were published in *Nature Communications*, addressing neuronal signals in vivo and in vitro. Among 212 other peer-reviewed publications, we have published the first review in the field of CI-based SiC growth (*Chemical Reviews*) and identified the origin of the lifetime limiting defect in bulk SiC (*Physical Review Letters*).

The grants of AFM have been partially invested in building strategic infrastructure for industry collaboration. A new XPS system was commissioned in 2012 with co-financing from the vice-chancellor. We have also upgraded our materials testing lab with strain test and a furnace. A new mass-energy analyzer for PVD-plasma characterization was commissioned.

We installed the advanced micro-Raman system capable of operating within the temperature range of 4-300K and under magnetic fields up to 5T.
Berggren received the Wallenberg Scholar and became an elected member of the Royal Swedish Academy of Sciences.

Docent Johana Rosén became KAW Academy Fellow.

Xavier Crispin was awarded the Tage Erlander prize, and the ERC starting grant.

Lars Hultman was named Editor-in-Chief for the journal VACUUM and Per Eklund Rapid Communications Editor of VACUUM.

The Organic Electronics team received major grants, incl. the SSF Framework Program in Material Science (Membrane Chromatography, together with Fredrik Höök, Chalmers), the VINNOVA-UDI (Printed Electronics for Internet of Things, with Acreo AB) and KAW project (Bioelectronics for plant science, together with Marcus Grebe, Umeå U.).

We were granted the EU-FP7-NMP project Life-Long Joints: Silicon Nitride Coatings for Improved Implant Function.

We were granted the EU FP7-PEOPLE-2012-IRSES International Research Staff Exchange Scheme PIRSES: Development of Nanotechnology-based Biosensors.

A VR Industry Graduate Student Project was granted for Ludvig Landälv of Sandvik Coromant AB to with the Thin Film Group at LiU.

We founded the companies: TiÅ, LumiSigns AB, n-WORKS AB, and REM AB.

Recently graduate PhD’s from AFM are employed by industry (e.g., Mattias Samuelsson at Impact Coatings AB, Jonas Lauridsen at SECO Tools AB, Lars Johnson at Sandvik AB; Axel Knutsson at Alfa Laval AB, Anders Eriksson at Balzer Oerlikon).

CeNano

The Centre in Nano Science and Technology (CeNano) is an organization within the Technical Faculty of Linköping University. The mission of CeNano is to strengthen and support the competence within nano science and nano technology of the faculty. This is made by gathering researchers with nano activities in the centre and by acting for increased collaborations and common projects in the nano realm. CeNano also acts for development and coordination of the graduate and under graduate education in this scientific area. Included in the mission of CeNano is also exposure of the faculty’s nano activities by seminars, actions for contact establishment, taking initiative to larger projects, etc.

THE BOARD OF CENANO:

- Lars Hultman, Chair
- Igor Abrikosov
- Per-Olof Holtz
- Olle Inganäs
- Per-Olov Käll
- Kajsa Uvdal, Director of CeNano

PROJECTS SUPPORTED CENANO IN 2012:

- Self-assembly of Anisotropy Nanostructure for Metal Enhanced Fluorescence and Plasmonically Triggered Drug Release PI: Daniel Aili
- Biocompatibility studies of engineered nanoparticles aimed for use in biomedical applications PI: Caroline Brommessen
- Nanoparticle-based localized surface plasmon resonance excitation for improved lateral resolution in SPR imaging of marine fouling organisms PI: Thomas Ederth
- Theoretical studies of the mixing thermodynamics of solid solutions of ScN with other mononitrides for the purpose of thermoelectric thin films PI: Per Eklund
- Boron Nitride – the ultimate substrate for Graphene PI: Anne Henry
- Synthesis and Characterization of Chiral Organic Nanostructures PI: Kenneth Järrendahl
- Nano-scale particles for efficient polymer-based light-emitting devices PI: Per-Olof Holtz
- Superhard Nanocrystalline Materials: Theory and Experiments PI: Ferenc Tasnadi
- Exploring ZnO Nanostructures Embedded in Polymers for Enhanced Performance in Light Emission and Photovoltaic Applications PI: Fengling Zhang
- Ultrabright Semiconducting Polymer Dots (Pdots) for Specific Cancer Cell Targeting PI: Xuanjun Zhang

HIGHLIGHTS

Exploring ZnO Nanostructures Embedded in Polymers for Enhanced Performance in Light Emission and Photovoltaic Applications

Fengling Zhang IFM, LiU

We prepared varied ZnO nanostructures. The light emission of the nanorods was studied by µ-PL in the temperature range of 4 – 300 K. The low temperature PL spectrum of high quality ZnO nanorods is solely dominated by NBE emission, which consists of several closely located peaks, attributed to the donor bound exciton emission (DoX)[Fig.1a]. The ZnO nanoray as electron acceptor was integrated in Hybrid solar cells (HSCs) with polymer Poly[2-methoxy-5-(2ethyl-hexyloxy)-1,4-phenylene vinylene] (MEH-PPV) as electron donor. The current density (J)-voltage (V) curves are shown in Fig.1b. The performance of the HSCs is mainly limited by large dimensions of ZnO nanostructures (diameter 100 nm and length 500 nm), which can be improved with reduced the dimensions of nanostructures by one order of magnitude.
Nanoparticle-based localized surface plasmon resonance excitation for improved lateral resolution in SPR imaging of marine fouling organisms Thomas Ederth IFM, LIU

Understanding how marine organisms explore and interact with surfaces is essential for the development of efficient and non-toxic antifouling coatings. In this project we take advantage of localized plasmons excited in surface-bound metal nanoparticles to improve the resolution in surface plasmon resonance imaging of spores and larvae of marine organisms and their interaction with surfaces.

Figure 1 LT PL spectrum of ZnO nanospikes (a) and illuminated J-V curves of the devices using different MEH-PPV/ZnO weight ratios (b).
Self-Organizing Nanoscale Coatings for Cutting Tools and Components
FunMat generates strategic knowledge for the deposition and structure evolution of new hard coatings used in wear protection of metal machining tools. The next generation of tools must withstand yet higher mechanical and thermal loads than those of today. We explore nanostructured ceramic coatings and push the frontiers of characterization techniques as well as computational methods.

HiPIMS Key Technology Platform for Cutting Tools and Low-friction Components
We explore hybrid HiPIMS Technology for advanced surface engineering. Target applications are for transition metal nitrides and resilient fullerene-like C-based coatings. We also develop coating/substrate adhesion processing. Expertise is provided on PVD deposition, plasma characterization, XPS, electron microscopy, nanotribology, as well as theoretical calculations.

New Nanoscale Sensor Materials & Application
Silicon carbide chemical sensors are commercialized for applications in harsh environment at temperatures below 400 °C. Applications at higher temperatures require improved contact materials. The conducting ceramic materials developed within FunMat offers a unique possibility for the silicon carbide sensors as well as other challenging sensor developments. Graphene epitaxially grown on SiC is developed as an ultra sensitive gas sensor for close to room temperature operation.

HIGHLIGHTS 2012
• Johanna Rosén appointed Wallenberg Academy Fellow
• Two spin-out companies (GraphenSiC and N-works)
• Four PhD theses (Doctors now working at Seco, LiU, Sandvik and Oerlikon Balzers)
• Five new PhD students (incl. one VR-industry PhD student with FunMat partner Sandvik)
• Dr Galia Pozina winner of the IVA –Royal Swedish Academy of Engineering Sciences "Mentor 4Research" Prize – a catalyst for commercialization
• Dr Naureen Ghafoor and Dr Per Eklund appointed Senior Lecturers
• Prof Lars Hultman winner of the Junior Faculty Prize 2012 at LiU for supporting the careers of junior researchers, thus creating a sustainable research environment
• 30 scientific publications in international peer-reviewed journals
• Expansion of strategic research infrastructure
• Industry – University mobility and job placements

Center Board Stage 3 (2012-2014)
Lennart Karlsson, SECO Tools AB (chair)
Birgit Jacobson, CEI-Europe AB (deputy chair)
Ann W Grant, Volvo Technology
William Salaneck, LiU
Peter Värbrand, LiU
Åke Öberg, ABB AB

Management Team
Prof. Lars Hultman (Head)
Prof. Anita Lloyd Spetz (Deputy Head)
Prof. Magnus Odén (Research Coordinator)
Ms. Therese Dannetun (Coordinator)
Prof. emerita Rositza Yakimova (Adviser)
Senior lecturer Per Eklund (leader Theme 1)

Partner Companies Stage 3 (2012-2014)
ABB AB, Corporate Research
Alstom Power
CemeCon AG
Ford Motor Company
Impact Coatings AB
Ionbond Sweden AB
Sandvik Tooling Sverige AB
LiLi-NFM

Linköping Linnaeus Initiative for Novel Functional Materials

LiLi-NFM is a coordinated laboratory for interdisciplinary research on advanced materials. It is supported by the Swedish Research Council (VR) for a 10-year period until 2016 by a Linnaeus Grant.

The research environment constitutes the backbone of materials research at Linköping. It consists of ~150 researchers from 9 divisions of IFM.

**Director:** Prof. Lars Hultman  
**Deputy Director:** Prof. Erik Janzén  
**Scientific Secretary:** Prof. Irina Yakimenko  
**Coordinator:** Ms. Camilla Karlsson

**Research Divisions and Principal Investigators:**

- **Computational Physics**  
  Prof. Sven Stafström
- **Functional Electronic Materials**  
  Prof. Weimin Chen  
  Prof. Irina Buyanova
- **Nanostructured Materials**  
  Prof. Magnus Ödén
- **Plasma & Coating Phys.**  
  Prof. Ulf Helmersson  
  Prof. Nils Brenning
- **Semiconductor Materials**  
  Prof. Erik Janzén  
  Prof. Peder Bergman  
  Prof. Per-Olof Holtz  
  Prof. Leif Johansson  
  Prof. Bo Monemar  
  Prof. Rositza Yakimova
- **Surface & Semiconductor Physics**  
  Prof. Göran Hansson,  
  Prof. Wei-Xin Ni  
  Prof. Roger Uhrberg
- **Surface Physics and Chemistry**  
  Prof. Mats Fahlander  
  Prof. Igor Abrikosov  
  Prof. Sergei Simak  
  Prof. Irina Yakimenko
- **Theory and Modelling**  
  Prof. Igor Abrikosov  
  Prof. Sergei Simak  
  Prof. Irina Yakimenko
- **Thin Film Physics**  
  Prof. Lars Hultman  
  Prof. Jens Birch  
  Prof. Esteban Broitman  
  Prof. Anne Henry  
  Prof. Joseph E Greene  
  Prof. Ivan Petrov  
  Prof. Michel Barsoum

**OBJECTIVE**

Our objective is in doing basic research to fundamentally understand the atomistic nature of materials synthesis, structure, and properties. We can thus extend the frontiers of materials and nanosciences to expand the scientific foundations for the development of materials that improve, e.g., the efficiency, environmental acceptability and safety in energy generation, conversion, transmission and use.

The core activity of LiLi-NFM is within the largest and most rapidly developing area of physics research worldwide. In fact, the understanding of materials is the fundamental driving force in natural science and basic engineering research. We focus on studies on the nature of epilayers, thin films, and nanoscale materials. Here, we are in the forefront regarding materials synthesis including wide-band gap materials (SiC, BN, AlN, GaN, ZnO), graphene, nanocomposites, superlattices, fullerene-like compounds, and organic molecular materials.
Our research concerns unsurpassed knowledge-based design of new functional materials for electronics, engineering, and the life sciences. We design material structures and explore outstanding phenomena. We also seek to discover novel phases.

GRAPHENE FLAGSHIP
Linköping University is taking part in the Graphene Flagship ramp-up stage, which is funded by EC within the FP7. The decision of funding is opening for the graphene researchers new horizons to bring this amazing material to revolutionary solutions in high speed electronics, medical diagnostics, space research, etc.

Researchers at IFM have the knowhow to produce one of the best graphene on silicon carbide worldwide. In November 2011 the first European company on epitaxial graphene (Graphensic AB) was founded as a spin off from LiU.

One of the goals of the Graphene Flagship is to bridge research and commercialization by creating new and improved graphene products to be implemented in advanced applications, which will bring added value to the society.

STRATEGY
It is our strategy for excellence to develop and integrate theory, simulations, and experiment. The philosophy for operating LiLi-NFM contains the following elements:

• Natural science and basic engineering research
• Strategic recruitments and tenure-track plans
• Intra-disciplinary excellence
• Inter- and multi-disciplinary modus operandi
• Strong national & international collaboration
• State-of-the-art laboratories
• Leading computational capacity
• Synergy and added value from collaboration

COMPETENCE PLATFORMS
LiLi-NFM supports the following competence platforms around which several profile projects are operated:

1. Materials Synthesis;
2. Materials Modeling;
3. Advanced Materials Analysis

RECENT STRATEGIC RECRUITMENTS

• Olle Kordina
• Per Eklund
• Jens Jensen
• Mathieu Linares
• Daniel Daganelund
• Martin Magnuson
• Weine Olovsson
• Henrik Pedersen
• Iris Pilch
• Fredrik Söderlind
• Daniel Söderström
• Jan Stehr

LILI-NFM SEMINARS SERIES
We organize open seminars. In 2012 presentations were given by Dr. R. Armiento, Dr. M. Magnuson, Dr. J. Jensen, Dr. V. Chirita (all IFM), and Dr. V.R.R. Medicherla (Institute of Technical Education and Research, Bhubaneswar, India).

SCIENTIFIC HIGHLIGHTS
Experimental and Theoretical Evidence of a Highly Ordered Two-Dimensional Sn/Ag Alloy on Si(111) [Jacek R. Osienski, H. M. Sohail, P. E. J. Eriksson, and R. I. G. Uhrberg, Phys. Rev. Lett. 109, 057601 (2012)].

The existence of a highly ordered, two-dimensional, Sn/Ag alloy on Si(111) is reported in this study. We present detailed atomic and electronic structures of the one atomic layer thick alloy, exhibiting a 2x2 periodicity. The electronic structure is metallic due to a free-electron-like surface band dispersing across the Fermi level. By electron doping, the electronic structure can be converted into a semiconducting state. A rotated Sn trimer constitutes the key structural element that could be identified by a detailed analysis of constant energy contours derived from the free-electron-like band.

Figure 1: Constant energy contours (up) and electronic band structure (bottom) of the 2D Sn/Ag alloy. In combination with a theoretical study, these data reveal the existence of rotated Sn trimers.

Spin polarization of nonmagnetic CdSe quantum dots (QDs) coupled to adjacent ZnMnSe diluted magnetic semiconductor (DMS) is investigated by CW and time-resolved magneto-optical spectroscopy under tunable laser excitation. Efficient enhancement in the degree of $\sigma^+_c$ circular polarization of photoluminescence from the CdSe QDs is observed under optical excitation at the $\sigma^-_c$-active exciton state of the DMS. The fact that the enhancement persists much longer than the exciton lifetime of the DMS rules out a role of the DMS excitons. A possible explanation is discussed in terms of antiferromagnetic coupling between the excitons in QDs and aligned Mn ions in DMS.

Nanoparticles in a size range of 10 to 40 nm were synthesized using a high power pulsed hollow cathode. It was shown that the size of the nanoparticles could be controlled by the pulse parameters, i.e., frequency, peak current and pulse width. By applying a high power pulse to a hollow cathode, a high degree of ionization of the sputtered source material is achieved. The growth process of nanoparticles in a pulsed, highly ionized plasma is discussed, and underlying mechanisms for controlling the growth process are proposed.

Density functional theory (DFT) calculations were performed in order to investigate the stability and the electronic structure of graphene-gold interfaces. Two configurations were studied: an Au cluster interacting with graphene and different polycyclic aromatic hydrocarbon (PAH) molecules, namely, C6H6 (benzene), C24H12 (coronene), and C54H18 (circumcoronene) adsorbed on Au(111). Nonlocal interactions were accounted for by using the semiempirical DFT-D2 method of Grimme. A limited set of calculations were also performed by using the first-principles van der Waals density functional method (vdW-DF). Adsorption distances around 3 Å and electronic charge transfer values of about \( (3-13) \times 10^{-3} \) e\(^-\) per C atom were predicted for all systems. No major changes resulting from the adsorption of the Au cluster were detected in the graphene's density of states. The DFT-D2 results involving the adsorption of the PAH molecules on Au show an estimated binding energy of 73 meV per C atom, as well as an electronic charge loss of 0.10 x 10^{-2} e\(^-\) per C atom, for an extended graphene sheet adsorbed on a Au surface. The modeling of the adsorption of C6H6 molecule on a Au surface suggests that the vdW-DF method provides more accurate results for the binding energies of such systems, in comparison to pure DFT calculations, which do not take the nonlocal interactions into account, as well as to simulations employing the DFT-D2 method.


Density functional theory (DFT) calculations were performed

We have discovered an anomalously high thermoelectric power factor in epitaxial ScN thin films, suggesting ScN-based materials as candidates for thermoelectric application. Our theoretical studies demonstrated that this is due to the defect states introducing sharp features in the electronic density of states, which would yield a large enhancement in Seebeck coefficient without reduction in electrical conductivity. Sc and N vacancies produce an asymmetric sharp feature in DOS of ScN. The other defects will move the position of the Fermi level (EF) depending on whether they are donors or acceptors, for example O, F, and Zr act as donors and C, Be, and Mg act as acceptor. Our results indicate a promising pathway to obtain high thermoelectric figure of merit in ScN-based materials by stoichiometry tuning and reduction of lattice thermal conductivity.


The origin of the anisotropic Seebeck coefficient (thermoelectric effect) in nanolaminated crystals is traced to anisotropies in element-specific electronic states by employing polarized angle-dependent x-ray spectroscopy. These results constitute experimental evidence explaining why the average Seebeck coefficient of Ti3SiC2 in polycrystals is negligible over a wide temperature range.
Surface morphology effects on the light-controlled wettability of ZnO nanostructures
The effect of surface morphology on the UV light-controlled wettability of ZnO nanostructures has been revealed [1]. The hydrophobicity state of the ZnO nanostructures is converted to superhydrophilicity after UV irradiation during ~5–30 min (Fig. 1), where smaller ZnO features on the surface yield a faster hydrophobicity-hydrophilicity transition. This is explained by the semiconductor nature of ZnO and its surface chemistry. The fastest and most prominent wettability change is obtained for ZnO nanosheaves: the contact angle changes from 124º to 5º after ~5 min of irradiation. Such effect is explained to be due to the small (~30 nm) needle tip diameter and their highly developed surface area. The results encourage the application of the ZnO nanostructures, particularly for the effective control of micro or nano-fluid motion, and enabling patterning hydrophilicity/hydrophobicity with photolithography. The observed features of ZnO can also be used for the design of microdevices, where the nature of a surface plays a key role on the mediation of protein adsorption or cell adhesion.

Figure 8: Change of the contact angle (θ) with time upon UV irradiation for ZnO nanostructures of diverse morphology. The insets are wettability images before irradiation (left) and after 5 min of UV irradiation (right).

The structural and electronic properties of an infinite h-AlN sheet were addressed by DFT calculations together with the implications for its network of selected defects, e.g., vacancies, anti-sites as well as C and Si impurities. Defects such as nitrogen vacancies and Si impurities lead to a breaking of the planar shape of the h-AlN sheet and in some cases to the formation of new bonds. The defects significantly change the band structure in the vicinity of the Fermi level in comparison to the band structure of the perfect h-AlN, which can be used for deliberately tailoring the electronic properties of individual h-AlN sheets.

Using n-type 4H-SiC epilayers irradiated by low energy (250 keV) electrons we were able to obtain the electron paramagnetic resonance (EPR) signals of the carbon vacancy (VC) without interference from other defects and determine its energy levels and negative-U properties. Combining EPR and deep-level transient spectroscopy (DLTS), the two most common defects in as-grown 4H-SiC—the Z$_{1/2}$ lifetime-limiting defect and the EH$_7$ deep defect—have been identified to be related to the double acceptor (2-|0) and single donor (0|+) levels of VC, respectively. The results clarify the long-standing issue on the origin of the lifetime limiting defect in bulk SiC.

Figure 9: Charge distribution iso-surfaces associated to the spin excess emerging from the SiAl defect incorporated in an h-AlN sheet.

Figure 10: Scheme of energy levels of VC at the hexagonal (h) and cubic (k) sites determined by photo-EPR and the Z$_{1/2}$ and EH$_7$ levels determined by DLTS.
LBB

Linköping Biosensors and Bioelectronics Centre (LBB)

STAFF
Director: Prof Anthony (Tony) Turner
Professors: Anthony Turner and Fredrik Winquist
Emeritus Professor: Ingemar Lundström
Associate Professor: Edwin Jager
Assistant Professors: Wing Cheung Mak, Ashutosh Tiwari and Valerio Beni
Ph.D. Students: Onur Parlak and Mohsen Golabi.
Research Fellows: Amy Gelmi and Hirak Patra
Visiting Researchers: Dr Raeann Gifford and Dr Douglas Holub
Visiting Scientists: Dr Masoud Meghardi; Dr Janno Torop; Dr Aysu Yarman; Dr Lokman Uzun;
Visiting PhD Students: Daniel Melling, Alina Sekeraytova, Jose Luise Sebastian Avila, Mabel Torrens del Valle, Leila Kashefi,
Najmeh Karimian, Jose G. Martínez and Roghayed Imani.
Diploma/Master Students: Nirul Masurkar, Nandim Nwora,
Aswathi Anto Anthony, Shalini Nagabooshnam, Aristide Ganci,
Ines Moreno, Nisar Ul Khalid, Jenny Orban, Swapneel Deshpande and Presty Mathew Merna.
Consultant: Dr Claes Nylander
Managing Editor: Dr Alice Tang
Administrative Staff: Anette Andersson

GENERAL INFORMATION
The Linköping Biosensors and Bioelectronics Centre (LBB) was set up in 2010, with the aim of bringing together the many competences, activities and resources at LiU that are already working on, or can bring valuable contributions to, the development of biosensors, biosensing, bioelectronic devices and relevant biomaterials and nanomaterials. The mission of the Centre is to improve the quality of life, health and the environment by the provision of distributed diagnostics and personalised analytical tools and therapies. Its remit encompasses implantable, minimally invasive and non-invasive techniques that may be wearable, used at the point of care or more widely distributed in the home or environment. Disease management is focused on cancer, cardiac diseases, infectious disease, diabetes and care of the elderly. The Centre’s principal tools are high level research, advanced teaching and the organisation of specialist conferences and workshops. During 2012, the Centre consolidated with the appointment of a number of seniors, including three in association with the Integrative Centre for Regenerative Medicine (IGEN). It also played a leading role in the management of Linköping Initiative in Life Sciences (LIST) and contributed to the strategic direction of New Tools for Health (HNV). The Centre further reinforced its role on the international stage in the rapidly expanding field of biosensors by the creation of several key international collaborations, organisation of two international workshops and several major conferences. Work at LBB today spans a full range of core technologies including: bioimaging and drug delivery; bio-inspired and bio-specific ligands; biointerfaces; biomaterials; biomolecular electronics; biosensors; chemical transducers; pre-clinical trials; printing and microfabrication; micro-actuators; nanomaterials and nanostructures; tissue scaffolds; smart materials and nanomaterials; therapeutics; and user interfaces and electronic design.

LBB’s seeks to harness the fundamental research activities and innovation at LiU to facilitate the creation of the next generation of bioelectronic devices and to support the national and worldwide development of the field. It is working closely with IGEN, headed by May Griffith, ACREO AB in Nortkoping and the Joint Research Centre for Biosensors in Singapore, headed by Bo Liedberg. Other key external collaborators are Cranfield University (UK), Helmholtz Centre for Environmental Research (UFZ) in Leipzig (Germany), Hacetette University (Turkey), Italian Institute of Technology in Pontedera, Jiangsu University (China), Manchester University (UK), National Institute for Materials Science Tsukuba (Japan), Potsdam University (Germany), Prince of Songkla University (Thailand), University of Calcutta (India), University of Florence (Italy), University of Wollongong (Australia), Wuhan Institute of Virology (China), Univeristat Rovira i Virgili (Spain), Zanjan University (Iran) and a number of well known companies.

BIOSENSOR AND BIOELECTRONICS
LBB is home to the principal journal in the field, Biosensors and Bioelectronics, published by Elsevier. Tony Turner is the Editor-In-Chief, Alice Tang is the Managing Editor and Ingemar Lundström is an Editor. The journal has the highest Impact Factor (5.602) for a research publication in the broad field of Electrochemistry, as defined by ISI, and is also the highest ranking journal in Sensors. The team handled over 3,000 submissions in 2012. www.elsevier.com/locate/bios

ADVANCED MATERIALS LETTERS (VBRi)
Ashutosh Tiwari is Editor-In-Chief of Advanced Materials Letters, published by VBRi Press, and Raeann Gifford is an Associate Editor. The journal seeks to promote studies of the structure, synthesis, characterisation and application of novel nanomaterials. http://amllett.org

BOOKS

THE WORLD CONGRESS ON BIOSENSORS
LBB organised the 22nd Anniversary World Congress on Biosensors, in association with Elsevier, in Cancun, Mexico 15-18 May 2012. The World Congress hosted ca. 700 delegates from all over the world and is the largest and most prestigious conference in the field. The Congress was chaired by its founder, Tony Turner, for the twelfth time. Seven delegates attended from the Centre, presenting 2 oral presentations and 5 posters. LiU achieved high visibility thanks to its large exhibition stand promoting the activities of the Centre and its close partners, New Tools for Health (HNV), GraphenSic and ACREO.
LABEL-FREE TECHNOLOGIES
The Centre organised the first international conference on Label-free Technologies, in conjunction with the University of Bonn and Elsevier, in Amsterdam, 1-3 November 2012. The conference was co-chaired by Tony Turner and Evi Kostenis (Bonn) and attracted over 200 delegates and 20 commercial exhibitions. The focus was on emerging techniques for drug discovery and life science research.

INTERNATIONAL WORKSHOPS
In advance of the World Congress on Biosensors in Cancun, LBB organised a one-day Summer School on Printed Biosensors and Electronics, aimed at providing an in depth and tutorial view of this specialist topic. The Summer School was sponsored by Elsevier (Amsterdam) and Erkon Inc. (USA) and attended by around 100 delegates. The Summer School was coordinated by Edwin Jager and Chaired by Tony Turner.

The Sweden-Japan Seminar on Nanomaterials and Nanotechnology (SJ-S-Nano), 10-11 September 2012, was a two-day bi-national event organised by LBB (Ashutosh Tiwari et al.) in collaboration with IGEN, LIST and the International Association of Advanced Materials (IAAM) at Campus Valla. It focused on recent advances in nanomaterials and nanotechnology and possibilities for further collaboration between Sweden and Japan. It very successfully incorporated additional presentations from colleagues in Tsukuba by video link on the second day. During the event, Hirak Patra was awarded the prize as “Best Young Scientist” from the International Association of Advanced Materials.

COST ACTIONS
MP1003: EUROPEAN SCIENTIFIC NETWORK FOR ARTIFICIAL MUSCLES
Edwin Jager is the national representative for Sweden on the management committee of this COST action, chairman of short term scientific missions (STSM) working group and vice-chairman of the medical devices and conference committee working groups. LiU received two visitors funded by STSM grants from this action in 2012. Dr. Janno Torop (University of Tartu, Estonia) and José Martínez (University of Cartagena, Spain).

COST/LIST SYMPOSIUM 2012
IFM hosted an international Workshop funded by COST action TD1003 entitled Bioinspired Nanotechnologies for Distributed Diagnostics, 26-27 April 2012, in conjunction with LIST. The symposium comprised 18 oral presentations interspersed with discussions and poster presentations. Ingemar Lundström and Tony Turner are the representatives for Sweden for this action and LiU hosted Dr Aysu Yarman (Potsdam Univ., Germany), funded by an STSM grant from this COST in 2012.

INTERNATIONAL AGREEMENTS
The Biosensors and Bioelectronics Centre signed an Erasmus exchange agreement with the University of Dundee (UK) for Masters students. Furthermore, the Centre consolidated its exchange agreement with Cranfield University (UK) by hosting two Master students for their final research project in 2012. Ashutosh Tiwari received a JSPS (Japan) Bridge Fellowship in 2012 for ‘A highly sensitive and reproducible nanobioreactor for the artificial kidney device’ and the Centre signed a collaboration agreement with the National Institute for Materials Science (NIMS) in Tsukuba, Japan.

SIMARC
Swedish Interdisciplinary MAgnetic Resonance Center

STAFF:
Director: Prof. Weimin Chen

Board:
Prof. Anders Lund, Linköping Univ., Chair
Prof. Weimin Chen, LiTH, Linköping Univ.
Prof. Per Hammarström, LiTH, Linköping Univ.
Prof. Erik Janzén, LiTH, Linköping Univ.
Prof. Eva Lund, HU, Linköping Univ.
Doc. Ann Magnusson, Uppsala Univ.
Prof. Bo Monemar, LiTH, Linköping Univ.
Prof. Einar Sagtuen, Oslo Univ. (Norway)

Senior scientists: Prof. Irina Buyanova, Prof. Uno Carlsson, Prof. Weimin Chen, Ass. Prof. Häkan Gustafsson, Prof. Per Hammarström, Prof. Erik Janzén, Prof. emeritus Anders Lund, Prof. emeritus Eva Lund, Prof. emeritus Bo Monemar, Dr. Sara Olsson, Prof. Nguyen Tien Son

Visiting scientists and post-docs (>1 month):
Dr. Alexandr Dobrovolsky, Dr. Daniel Dagnelund, Prof. Mikael Lindgren, Prof. Galyna Rudko, Dr. Jan Stehr, Dr. Igor Vorona

PhD students:
Emelie Adolfsson, Axel Israelsson, Jan Beyer, Shula Chen, Stanislav Filippov, Mattias Karlsson, Yuttapoom Puttisong, Xuan Thang Trinh.

Administrative/Technical staff:
Susanne Andersson, Anna-Karin Stál, Arne Eklund

SUMMARY OF ACTIVITIES
The research activities at SIMARC cover several areas of various disciplines, including materials science, chemical physics, chemistry, radiation physics and medical science. The materials studied include advanced semiconductor materials, organic materials for dosimetry and biochemical materials.
Important defect issues and recombination processes in semiconductor materials

The goal is, by electron paramagnetic resonance (EPR) and optically detected magnetic resonance (ODMR), to identify chemical nature and geometrical structure of defects, impurities and dopants that are important in semiconductor materials and nanostructures. The activities in this area during 2012 were focused on: (i) Ga(In)NAs and GaNP dilute nitrides; (ii) SiC; and (iii) ZnO.

**EPR dosimetry**

The aim is to improve EPR dosimetry (ionising radiation dose measurements) to be a competitive dosimetric method for applications in radiation therapy. We worked with optimization of measurement precision and accuracy in dose measurements by development of new dosimeter read-out protocols and dosimeter calibration protocols. We were also searching for new dosimeter materials with higher sensitivity and better tissue equivalence with respect to attenuation and scattering of ionizing radiation. We are currently clinically evaluating a lithium formate EPR dosimeter system for dosimetry in special measurements situations such as dosimetry in intensity modulated radiation therapy (IMRT) and brachytherapy with electronic sources i.e. a micro X-ray tube. Further the robust design and high stability of the dosimeters were used for verification of the whole radiotherapy chain.

**Retrospective dosimetry by means of EPR spectroscopy**

EPR spectroscopy measurements of chewing gums and sweeteners sorbitol and xylitol have been performed in order to optimize their use as retrospective dosimeters. We participated in an international intercomparison on retrospective dosimetry of Touch Glass in mobile telephones. Radical identification, transitions, stability, dose response and light dependence have been investigated. Retrospective dosimetry on finger nails has been performed with a focus on the preparation procedures to avoid mechanically induced signals. First attempts were made on imaging of the dose distribution in tooth enamel by imaging of simple geometries of enamel grains in paraffin and carbonated hydroxyapatite.

**Medical applications of EPR imaging (EPRI)**

Research aiming to use EPRI for medical applications such as: (i) imaging of radical distributions in atherosclerosis for a better understanding of the role of reactive oxygen species (ROS) in atherosclerosis; (ii) imaging of radical distributions for experimental verifications of calculated dose distributions in radiation therapy of cancer, e.g. narrow beam dose distributions and interface dose distributions; (iii) imaging and spectroscopy of spin-labelled amyloid proteins involved in degenerative diseases.

**Education activities**

We have also been actively involved in undergraduate and graduate education. During 2012, the courses in “Semiconductor Technology” (TFYA30), “Perspectives on Physics” (TFFM12), “Experimental Physics” (TFFMoS), “Project work” (TGZD20) and “Magnetic resonance characterization of defects in semiconductors” were given.

**HIGHLIGHTS**

Defect properties of ZnO nanowires revealed from an ODMR study. ODMR complemented by photoluminescence measurements.
Publications 2012

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Theses

Doctoral Theses

LÖGDBERG, FRIDA: Population dynamics in variable environments– impacts of noise colour and synchrony
Dissertation No 1416 (13 January 2012)

WIRÉN, ANDERS: Correlated selection responses in animal domestication: the behavioural effects of a growth QTL in chickens
Dissertation No 1413 (20 January 2012)

ANDERSSON, VIKTOR: Electron tomography and optical modelling for organic solar cells
Dissertation No 1414 (3 February 2012)

JAKOSSON, MATTIAS: Monte Carlo studies of charge transport below the mobility edge
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ROGSTRÖM, LINA: High temperature behaviour of arc evaporated ZrAIN and TiAIN thin films
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BEYER, JAN: Spin properties in InAs/GaAs quantum dot based nanostructures
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KANERED, LINDA: Dynamics of ecological communities in variable environments – local and spatial processes
Dissertation No 1431 (4 April 2012)

HÅKANSSON, NINA: Network analysis and optimization of animal transports
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LENNARSSON, JENNY: Networks and epidemics – impact of network structure on disease transmission
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SANDGREN, VERONICA: Design and Synthesis of Inhibitors Targeting BACE-1, an Aspartic Protease Involved in the Pathogenesis of Alzheimer’s Disease
Dissertation No 1436 (27 April 2012)

VASILIAUSKAS, REMIGIJUS: Sublimation Growth and Performance of Cubic Silicon Carbide
Dissertation No 1435 (3 May 2012)

FYNER, TIMMY: Synthesis of Orthogonally Functionalized Oligosaccharides for Self-assembled Monolayers and as Multimodal Tools in Chemical Biology
Dissertation No 1442 (11 May 2012)

HUNG-HSUN LEE: Structural Studies of Oligo (ethylene glycol) – Containing Assemblies on Gold
Dissertation No 1446 (31 May 2012)

SETZER, MALIN: The decline of great Arctic charr in Lake Vättern – empirical and theoretical analyses of suggested causes
Dissertation No 1447 (1 June 2012)

STENETG, PETER: Development of molecular dynamics methodology for simulations of hard materials
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EKHOLM, MARCUS: Theoretical descriptions of complex magnetism in transition metals and their alloys
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HELLMAN, OLOF: Thermal properties of materials from first principles
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SAMUELSSON, MATTIAS: Fundamental aspects of HiPIMS under industrial conditions
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LUNDSKOG, ANDERS: Controlled growth of hexagonal GaN pyramids and InGaN QDs
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SEHATI, PARISA: Influence of intermolecular order at the interfaces
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GABRIELSSON, ROGER: Electroactive Conjugated Polyelectrolytes Based on EDOT
From synthesis to Organic Electronics
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IQBAL, ZAFAR: Optical Sensing With an Ordinary Mobile Phone
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KNUTSSON, AXEL: Thermal stability and mechanical properties of TiAIN-based multilayer and monolithic coatings
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JUNAID, MUHAMMAD: Magnetron Sputter Epitaxy of GaN: Epilayers and Nanodots
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Licentiate Theses

BERGSTRÖM, Gunnar: Exploring the SPR methodology for monitoring of critical attributes in toxicity testing and bioproduction
Thesis No 1517 LIU-TEK-LIC-2012:2

KHROMOV, SERGEY: The effect of Mg doping on optical and structural properties of GaN
Thesis No 1520 LIU-TEK-LIC-2012:5

SCHMIDT, SUSANN: Carbon based thin films prepared by HiPIMS and DCMS
Thesis No 1521 LIU-TEK-LIC-2012:6

SJOÖVIST, JONAS: Luminescence properties of flexible conjugated dyes
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ZUKAUSKAITE, AGNĖ: Metastable YAIN and ScAIN thin films: growth and characterization
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GÖRANSSON, ANNA-LENA: The Alzheimer AB Peptide: Identification of Properties Distinctive for Toxic Prefibrillar Species
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PUTTISONG, YUTTAPOOM: Spin-dependent recombination in Ga(In)NAs alloys
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CHEN, SHULA: Excitonic effects in ZnO
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AIJAZ, AZIM: HiPIMS-based Novel Deposition Processes for Thin Films
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MOKUTE AURELIJA: Thin Film Synthesis and Characterization of New MAX Phase Alloys
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Ex-2613 FRANSSON, MARCUS: Stability study of transthyretin at different temperatures using urea denaturation and tryptophan fluorescence spectroscopy


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Ex-2625 FALLAHSHAHRUDI, AMIR: Domestication related genotype on ADRA2C - a determinant of feature response in chickens?

Ex-2626 HUQ, MD. NAZMUL: The genetic basis of a domestication trait in the chicken: mapping quantitative trait loci for plumage colour

Ex-2627 KIM, SUNGHEE: Olfactory discrimination ability of South African fur seals (Arctocephalus pusillus)

Ex-2629 MATHEW, BINU: T regulatory cells (Tregs) from interferon gamma (INF-γ) deficient mice contribute to a reduction in the formation of auto-antibodies in mice exposed to mercury chloride

Ex-2630 MUSA, NAJIHAN: Using sex pheromone and a multi-scale approach to predict the distribution of a rare saproxylic beetle

Ex-2631 NYCÅRDS, SOFIA: Importance of habitat quality and landscape factors for a monophasic shield bug on a rare host plant

Ex-2632 ODHAMMAR, ANNA M E: Olfactory sensitivity of spider monkeys (Ateles geoffroyi) for predator odours

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Ex-2638 RAVICHANDRAN, PRAVIN: Is the vasodilatory effect of nitric oxide on the brood patch microcirculation enhanced during broodiness in Red Junglefowl (Gallus gallus) and Zebra Finch (Taeniopygia guttata)?

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Ex-2642 THERNSTROM, TAINA: Maximum price paid in captive Bush dogs (Speothos venaticus)

Ex-2643 URIO, FLORENCE: EBV immortalization and characterization of malaria specific B cells from immune donors

Ex-2644 EKSTRÖM, ANDREAS: Metabolic implications of having a small heart: Indications of hypometabolism and genetic alterations in glycolytic metabolism in the Ornate Tinamou, Nothroprocta ornata

Ex-2647 GASPARINI, ISABELLA: Cardiorespiratory responses upon increased metabolism in the Ornate Tinamou, Nothroprocta ornata

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Ex-2649 SARRAFCHI, AMIR: Equine stereotypic behavior as related to horse welfare: A review

Ex-2652 BERGNER, ADAM: Studier av habitatval och restrukturerings hos vassängare (Locustella luscinioides) i Takern

Ex-2653 BERGWAHL, CAROLINE: The domestication effects on social support in chickens (Gallus gallus)

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Ex-2660 JONSSON, JOHAN: The effect of rope and an activation ball on the performance of harmful social behaviors in pigs

Ex-2661 KATAJAMAA, REBECCA: Effects of domestication on social support in chickens (Gallus gallus)

Ex-2662 LINDBLOM, EMELIE: Traits and behaviour affecting social status in red junglefowl (Gallus gallus) hens

Ex-2663 LUNDBERG, MALIN: Habitat preferences of tjeckskål malarmussla (Unio crassus) med avseende på vattendjur och beskuggning

Ex-2664 MOLIN, JOHAN: Predation on evertebrater under tidig vår i sjön Takern

Ex-2665 NILSSON, EMMA: The effects of an activity ball and ropes on pigs’ behaviours

Ex-2666 NILSSON, SARA: Use of space in captive Siberian tigers

Ex-2670 NILSSON, SOFIA: Effects of stress on fowl and their need for social support

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Ex-2672 KETARAWONG, ANNOP: Growth and characterization of graphene on 4H-SiC(0001)

Ex-2673 PETTERSSON, ELIN: Vilken preferens har tjockskalig malarmussla (Unio crassus) för bottensubstrat och vattenhastighet i Storån, Östergötland?

Ex-2675 SONELIN, SARAH: Effekter av luftföroreningar på lavar och grönalger på lind i Norrköpings kommun

Ex-2677 VENNERHOLM, LINN: Ontogeny of personality in red junglefowl chicks

Ex-2678 WEDDFELT, ERIKA: Recycling potential of phosphorus in food – a substance flow analysis of municipalities

Ex-2679 LE MOINE, REBECCA: The land use cover changes from 1992 to 2011 in Karbi Anglong, Assam, India

Ex-2680 SARRAFCHI, AMIR: Olfactory sensitivity of human subjects for six predator odorants

Ex-2681 SCHARIS, INGER: Cross-fostering in Grey wolves (Canis Lupus)

Ex-2682 LUNDBERG, GUSTAF: Core Level Binding Energy Shifts in a random AgPd alloy using the Exact Muffin-Tin Orbital method

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