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The Department of Physics, Chemistry and Biology (IFM) hereby presents its 44th consecutive progress report since the start in 1970. The report contains a description of activities in research and education within the department and in collaborations and it 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 funding 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 2014, 27 doctoral and 16 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 cover image is a colorized SEM image of Zinc Oxide nanorods decorated with copper nanoparticles giving it the appearance of marine coral (a “nanocoral”). Due to its heterogeneity and high specific surface area, this new type of material has many potential applications, for example as forming the basis for new catalytic materials. The image was taken by Robert Boyd, Plasma and Coatings Group at IFM.

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

Please 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

Financial Administrator

Inger Johansson

HR manager

Louise Gustafsson

Principal Research Engineer

Bengt Andersson/Henrik Jacobsson

Department Board

Members

Göran Hansson, Chairperson
Igor Abrikosov, Teacher Representatives
Kenneth Järrendahl, Teacher Representative
Peter Nilsson, Teacher Representative
Johanna Rosén, Teacher Representative
Uno Wennergren, Teacher Representative
Susanne Andersson, Techn/adm. Representative
Mattias Tengelius, PhD stud. Representative
Martin Eriksson, PhD-student Representative
Jonas Hartman, Student Representative

Deputy Members

Per Jensen
Karin Enander
Magnus Odén
Elke Schweda
Bjorn Wallner
Jeanette Nilsson

Other Members

Louise Gustafsson
Inger Johansson

Scientific Areas

Divisions

Applied Physics

Biology
Ecology, Molecular Genetics, Zoology

Chemistry

Material Physics
Functional Electronic Materials, Nanoscience Engineering, Nanoscale Materials, Plasma and Coatings Physics, Semiconductor Materials, Surface and Semiconductor Physics, Thin Film Physics

Theory and Modelling
Bioinformatics, Theoretical Biology, Theoretical Chemistry, Theoretical Physics

Study Programmes

Ph.D. studies

Biology

Chemistry

Physics – Engineering

Physics – Natural Science

Physics – Measurement Technology

Research Centres

AFM

Biosensors and Bioelectronics Centre

CeNano

FunMat

LiLi – NFM

MS²E

SIMARC
Undergraduate Teaching

**AREA**  
Biology  
Chemistry  
Physics  
Physics – Measurement Technology  

**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  
Magdalena Svensson  
Magnus Johansson  
Magnus Boman  

Graduate Teaching

**IFM Graduate Programme**  
Forum Scientium  
Agora Materiae  

**Research Divisions**

**Scientific Branch of Applied Physics**  
Applied Optics  
Applied Sensor Science  
Biomolecular and Organic Electronics  
Biosensor and Bioelectronics  
Biotechnology  
Chemical and Optical Sensor Systems  
Molecular Surface Physics and Nanoscience  
Molecular Physics  
Surface Physics and Chemistry  

**Scientific Branch of Biology**  
Ecology  
Molecular genetics  
Zoology  

**Scientific Branch of Chemistry**  
Biochemistry  
Inorganic Chemistry  
Molecular Biotechnology  
Organic Analytical Chemistry  
Organic Chemistry  
Physical Chemistry  
Protein Chemistry  

**Scientific Branch of Material Physics**  
Functional Electronic Materials  
Nanoscale Engineering  
Nanostructured Materials  
Plasma & Coatings Physics  
Semiconductor Materials  
Surface and Semiconductor Physics  
Thin Film Physics  

**Scientific Branch of Theory and Modelling**  
Bioinformatics  
Theoretical Biology  
Theoretical Chemistry  
Theoretical Physics  

**Research Divisions**

**Director of Studies**  
Agneta Johansson  
Agneta Johansson  
Agneta Johansson  
Wei-Xin Ni
Economy

**Operating Income (MSEK)**

<table>
<thead>
<tr>
<th></th>
<th>2014</th>
<th>2013</th>
<th>2012</th>
</tr>
</thead>
<tbody>
<tr>
<td>University allocations for teaching</td>
<td>83</td>
<td>88</td>
<td>87</td>
</tr>
<tr>
<td>University allocations for research</td>
<td>170</td>
<td>168</td>
<td>168</td>
</tr>
<tr>
<td>External sources of income</td>
<td>224</td>
<td>204</td>
<td>193</td>
</tr>
<tr>
<td>Total</td>
<td>477</td>
<td>460</td>
<td>448</td>
</tr>
</tbody>
</table>

**Operating Expenses (MSEK)**

<table>
<thead>
<tr>
<th></th>
<th>2014</th>
<th>2013</th>
<th>2012</th>
</tr>
</thead>
<tbody>
<tr>
<td>Expenses for staff</td>
<td>263</td>
<td>253</td>
<td>237</td>
</tr>
<tr>
<td>Expenses for premises</td>
<td>69</td>
<td>70</td>
<td>69</td>
</tr>
<tr>
<td>Other operating expenses</td>
<td>125</td>
<td>117</td>
<td>116</td>
</tr>
<tr>
<td>Depreciation</td>
<td>35</td>
<td>34</td>
<td>26</td>
</tr>
<tr>
<td>Total</td>
<td>492</td>
<td>474</td>
<td>448</td>
</tr>
</tbody>
</table>

**Change in Capital for the Year (MSEK)**

<table>
<thead>
<tr>
<th></th>
<th>2014</th>
<th>2013</th>
<th>2012</th>
</tr>
</thead>
<tbody>
<tr>
<td>Balanced capital January</td>
<td>46</td>
<td>60</td>
<td>65</td>
</tr>
<tr>
<td>Balanced capital December</td>
<td>31</td>
<td>46</td>
<td>66</td>
</tr>
</tbody>
</table>

**External Sources of Income (MSEK)**

<table>
<thead>
<tr>
<th>External Source</th>
<th>2014</th>
<th>2013</th>
<th>2012</th>
</tr>
</thead>
<tbody>
<tr>
<td>Swedish Research Council, VR</td>
<td>64</td>
<td>64</td>
<td>54</td>
</tr>
<tr>
<td>Other Research-funding agencies, e.g. Vinnova, Formas</td>
<td>24</td>
<td>18</td>
<td>18</td>
</tr>
<tr>
<td>Research foundations, e.g. SSF</td>
<td>23</td>
<td>22</td>
<td>20</td>
</tr>
<tr>
<td>Other private foundations, e.g. Wallenberg</td>
<td>55</td>
<td>47</td>
<td>30</td>
</tr>
<tr>
<td>Funding from the European Union</td>
<td>28</td>
<td>23</td>
<td>32</td>
</tr>
<tr>
<td>Other sources of funding</td>
<td>18</td>
<td>20</td>
<td>26</td>
</tr>
<tr>
<td>Contract research</td>
<td>8</td>
<td>10</td>
<td>14</td>
</tr>
<tr>
<td>Total</td>
<td>220</td>
<td>204</td>
<td>193</td>
</tr>
</tbody>
</table>
Personnel Situation 2014

<table>
<thead>
<tr>
<th>Position</th>
<th>2014</th>
<th>2013</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Women</td>
<td>Men</td>
</tr>
<tr>
<td>Professor</td>
<td>10</td>
<td>47</td>
</tr>
<tr>
<td>Associate Professor</td>
<td>1</td>
<td>4</td>
</tr>
<tr>
<td>Adj Professor</td>
<td>0</td>
<td>6</td>
</tr>
<tr>
<td>Guest Professor</td>
<td>0</td>
<td>6</td>
</tr>
<tr>
<td>Adj Lecturer</td>
<td>3</td>
<td>4</td>
</tr>
<tr>
<td>Research Fellow</td>
<td>5</td>
<td>1</td>
</tr>
<tr>
<td>Assistant Professor</td>
<td>15</td>
<td>33</td>
</tr>
<tr>
<td>Postdoctor</td>
<td>21</td>
<td>43</td>
</tr>
<tr>
<td>Other researcher</td>
<td>10</td>
<td>42</td>
</tr>
<tr>
<td>PhD student</td>
<td>46</td>
<td>87</td>
</tr>
<tr>
<td>Administrator</td>
<td>24</td>
<td>1</td>
</tr>
<tr>
<td>Engineer</td>
<td>5</td>
<td>15</td>
</tr>
<tr>
<td>Coordinator/Environm.</td>
<td>1</td>
<td>0</td>
</tr>
<tr>
<td><strong>Total</strong></td>
<td>141</td>
<td>259</td>
</tr>
</tbody>
</table>

New Professors 2014

Martijn Kemerink obtained his PhD in Applied Physics from Eindhoven University of Technology (TU/e, the Netherlands) in 1998 on the topic of Many-body Effects in III-V Semiconductor Heterostructures. Between 1998 and 2003 he worked as Fellow of the Royal Netherlands Society of Arts and Sciences on scanning tunneling microscope induced luminescence and spectroscopy on inorganic and organic semiconductors. In 2003 (2009) he became assistant (associate) professor in the group Molecular Materials and Nanosystems (M2N) at the TU/e. Within M2N he set up research activities on charge transport and device physics of organic semiconductors. Devices looked at include solar cells, thermogenerators, light emitting electrochemical cells and memories.

Since January 2014 Martijn is full professor in Applied Physics at the Department of Physics, Chemistry and Biology (IFM) at Linköping University, Sweden, and chairs the research division ‘Complex Materials and Devices’ (CoMaDe) which at the moment is embedded in the division Chemical and Optical Sensors (Cheops). The research in CoMaDe focusses on novel, predominantly organic, materials and devices in which multiple time, energy and/or length scales are important. Targeted device functionalities are harvesting of (renewable) energy from e.g. (waste) heat or sunlight, electrical data storage etc. To this end, a variety of device architectures including diodes, transistors and ratchets are investigated.

Currently, Martijn published over 125 peer reviewed papers and has an h-index of 30.

Fengling Zhang received her PhD from Changchun Institute of Physics, Chinese Academy of Sciences in 1998 on Organic light-emitting diode. Then she joined Department of Applied Chemistry at Osaka University, Japan as a postdoc. In 2000, she came to Department of Physics, Chemistry and Biology (IFM), Linköping University as a postdoc and began working on Polymer Solar Cells. Her research covers optimizing new polymers, exploring new device structures and investigating the factors governing the photovoltaic performance of polymer solar cells. She pioneers in ITO-free solar cells, soluble interfacial layer modifying cathode, vacuum free inverted solar cells and controlling morphology with mix solvents. 2007 she became a Docent. She is a VINNMER Fellow. Since 2009, her research extended to ZnO hybrid solar cells, soluble small molecule solar cells and fundamental study the mechanism of organic solar cells. April 2014, she became a professor at LiU. She is working on solar-powered organic electrochromic smart windows, exploring detecting bioluminescence with organic photodetectors and green biodegradable organic solar cells.

Since 2001, she published 115 peer reviewed papers with an h-index of 43. She was awarded the World’s Most Influential Scientific Minds by Thomson Reuters in 2014, which made a big contribution to LiU’s ranking in ARWU2014.

http://www.liu.se/liu-nytt/arkiv/nyhetsarkiv/1.579883?l=en
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 system**

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 objective areas and objectives. 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 action plan for 2013–2015 was decided by the IFM board in June 2013 and revised in August 2014 and consists of an action plan with environmental objectives and measures needed to be taken. The environmental work has been presented in the local co-operation group during the year.

**Environmental Action Plan at IFM 2013–2015**

The IFM action plan is based on the LiU environmental objectives. The objectives are organised according to environmental objective areas and are to be accomplished by 2015-12-31.

**Expanding knowledge of the environmental dimension of sustainable development**

1. The internal LiU environmental work will be communicated to all employees and students at campus, by 2015 at the latest.
   Measures IFM will take are improvement of the internal environmental website. Work with the website was initiated during 2014. Environmental- and laboratory safety information shall be introduced as a standing item in the IFM weekly newsletter and 14 of 40 newsletters contained environmental- or laboratory safety information during 2014.

2. Reduce the electricity consumption at LiU by 5 % per employee/student by 2015 compared with 2011.
   Measures IFM will take are e.g. participate in the LiU campaign to reduce the energy use, an inventory and evaluation of the energy save potential at IFM and information to all employees about the energy consumption annually. Work to fulfill measures was not accomplished during 2014.

3. Energy consumption of computers and servers at LiU will be measured and reduced, following a realistically set target, during the period 2013–2015.
   IFM participated in the LiU inventory of the number of computers, servers and screens during 2013. At IFM there are 2189 computers and 1351 screens available. Number of servers has not been reported.

4. The proportion of air travel consisting of journeys shorter than 500 km will be reduced, and in relation to long distance air travel, the CO₂ emissions will be less than 2 % of the total CO₂ emissions from air travel by 2015 at the latest.
   Measures IFM will take are e.g. information to employees about available travel-free meeting alternatives at IFM and LiU, information about environmental friendly travelling and the LiU travel handbook. During 2013, IFM received funding from the University climate compensation fund together with two other Departments at LiU to compensate for increased costs when traveling by other transportation means than by air. During 2014 one application for compensation was submitted to the environmental coordinator. More information is needed and will continue until April 2015.

5. The use of private cars for business purposes will be reduced and the use of LiU-Service cars will increase. The use of private cars for business purposes will be maximum 20 % of the total use of cars for business travel by 2015 at the latest.
   During 2014 information efforts have been given employees in weekly newsletter about LiU-Service rental cars and bicycles. Information efforts will continue during 2015.

**Streamlining the use of natural resources**

6. Reduce the consumption of copying/printer paper per employee and student by 10 % by 2015 compared with 2011.
   Measures IFM will take are e.g. participate in the LiU campaign form employees to reduce paper consumption and follow up the paper consumption at IFM and inform about it. Work to fulfill measures wasn’t accomplished during 2014.

7. Reduce the amount of waste that is incinerated from LiUs facilities by 10 % between 2013 and 2015.
   Measures IFM will take are information to employees about the waste recycling system and improve the information available on the IFM intranet. Work to fulfill measures wasn’t initiated during 2014.

**Minimizing the spread of harmful and infectious substances from the facilities**

8. Harmful substances in LiU’s IT equipment will be phased out continuously.
   An inventory of number of computers, tablets, screens and smartphones at IFM was made 2013. For information see objective three above. At IFM there are also 33 tablets available. Number of smartphones couldn’t be obtained.

9. Replace or reduce the use of substances harmful to health or to the environment in laboratory environments, where possible, by substitutions and changes to methods during the period 2013–2015.
   Measures IFM will take are e.g. follow up the substitution survey from 2012 and inform employees to investigate the possibility to replace/reduce the use of environmental- and health hazardous chemicals. Work to fulfill measures was initiated during 2014.
Equal Opportunities

IFM believes that equal opportunities are important for both students and employees. The department has therefore assigned the responsibility of equal opportunities to a group that during 2014 had following members: Lejla Kronbäck (administrative staff), Anna Sundin (administrative staff), Simona Eles (technical staff), Chun-Xia Du (technical staff), Ulf Frykman (technical staff), Mia Eriksson (PhD-student), Göran Hansson (prefect), Agneta Johansson (director of studies) and Uno Wennergren (professor).

The group’s aim is 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 discrimination grounds; gender equality and gender issues, ethnicity and religion or other belief systems, disabilities, sexual orientation and gender identity and victimisation, 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.

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.

During 2014 IFM hosted numerous visits by youth from, among others, Katrineholm, Norrköping, Vimmerby, Gränna, Grantham (Pennsylvania, USA), and Linköping, and we have offered exciting demonstrations and lectures on topics related to physics, biology and chemistry.

IFM participates in the annual activity Teknikåttan, which is a national competition in natural science and technology for pupils in eight grade, involving more than 500 schools and universities. This year there were four school classes in Linköping’s regional competition at Linköping University.

SUMMER SCHOOL

LiTH arranges a summer school, “Sommarveckan”, for pupils in elementary school, at the age of 14-15 years, who want to learn more about natural science and technology.

In 2014, the event consisted of five days with different themes. The week started with a day about physics at IFM. The remaining days included computer science, visualisation, biology, chemistry and technology. There were 50 participants, mainly from the region, but also from Gotland and Västmanland.

During the physics day the pupils were shown a demonstration of different phenomena occurring at low temperatures, such as superconductivity. One popular moment was when they got to crush roses cooled by liquid hydrogen to low temperatures. There also was a showroom with different demonstrations of ordinary everyday physical phenomena. Another popular event during the day was a tour in some of the research facilities, including short presentations of research projects.

MAY MINGLE

In May we have a popular activity targeting 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 MAI.

POPULAR SCIENCE WEEK

In October we participated in a Popular Science week for the general public. The IFM-professor Per Jensen initiated this event in 2005, and the interest is steady growing since then.
Photos from the summer school “Sommarveckan”.

The success of the initial Popular Science day has led to a larger three-day arrangement involving fields from the entire university, the Popular Science week, with about 2000 visitors. IFM participated 2014 with exhibitions given by PhD students as well as lectures by senior researchers on Alzheimer’s disease, species conservation, eutrophication as well as material physics and nanophysics.

IN-JOB TRAINING FOR HIGH SCHOOL TEACHERS

In October the Chemistry department hosted an in-job training day for high school teachers active in Östergötland. The program consisted of lectures from active researchers, a tour of the research lab facilities and a fruitful discussion between highschool teachers and university teachers on topics of mutual interest concerning chemistry education.

OPEN HOUSE DAYS

During the annual Open House days arranged by Linköping University, IFM participated with hands-on exhibitions. These days aim to inspire teachers and pupils from upper secondary school and encourage the pupils to head for higher education.
The undergraduate education given by the Department of Physics, Chemistry and Biology (IFM) had four main divisions 2014.

- Physics (Director of Studies: 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: Magdalena Svensson)

These divisions have in turn subprograms.
Physics

STAFF

**Director of studies:** Magnus Johansson

**Administrative assistants:** Agne Virsilaite Maras

**Technical staff:** Hasan Dzuho and Jonas Wissting

**Course leaders:** Björn Alling, Rickard Armiento, Hans Arwin, Jens Birch, Magnus Boman, Irina Buyanova, Valeriu Chirita, Marcus Ekholm, Per Eklund, Fredrik Eriksson, Jens Eriksson, Mats Eriksson, Ragnar Erlandsson, Urban Forsberg, Carl Hemmingsson, Magnus Johansson, Kenneth Järrendahl, Fredrik Karlsson, Peter Münger, Son Tien Nguyen, Wei-Xin Ni, Weine Olovsson, Plamen Paskov, Johanna Rosén, Per Sandström, Kostas Sarakinos, Sergei Simak, Bo Sernelius, Mikael Syväjärvi, Niclas Solin, Ferenc Tasnadi, Roger Uhrberg, Sergy Valyukh, Chariya Virojanadara, Irina Yakimenko

**Assistant lecturers:** Peter Andersson, Robert Pilemalm

**Teaching assistant:** Maria Pihl

In our division, we are responsible for physics courses on the following 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 (80)

**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. Starting from 2014, the third-year students on the Y(Yi)-program can choose to make a Bachelor Project in Applied Physics offered at our division. 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 3 profiles; related to our division is Biomedical engineering materials (Thomas Edelth).

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, on the Master’s Programme in Physics and Nanoscience (MFYS), on the International Master’s Programmes in Materials Science and Nanotechnology (MSN), and, to a minor extent, Biomedical Engineering (BME) and System on Chip (SoC). Contact persons in our division are Marcus Ekholm (FyN, MFYS) and Wei-Xin Ni (MSN).

Below is a list of the courses given by our division in 2014.

**TUITION IN PHYSICS**

**Basic courses:**

- Applied Physics - Bachelor Project (Y, Yi), 16hp
- Electromagnetic Field Theory (FyN, Y, Yi), 8hp
- Electromagnetism - Theory and Applications (IT), 8hp
- Electromagnetism - Theory and Applications (MED), 6hp
- Engineering Mechanics (D), 6hp
- Engineering project (MED, Y, Yi), 6hp
- Models in Physics (IT), 8hp
- Modern Physics (MED), 6hp
- Modern Physics I (FyN, Y, Yi), 4hp
- Modern Physics II (FyN, Y, Yi), 4hp
- Nano Scientific Project (FyN), 6hp
- Nanotechnology (BME, FyN, MFYS, MSN, 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), 6hp
- 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, 6hp
- Analytical Mechanics, 6hp
- Analytical Methods in Materials Science, 6hp
- Classical Electrodynamics, 6hp
- Chaos and Nonlinear Phenomena, 6hp
- Computational Physics, 6hp
- Elementary Particle Physics, 6hp
- Experimental Physics, 6hp
- Material Optics, 6hp
- Mathematical Methods of Physics, 6hp
- Nano Physics, 6hp
- Optoelectronics, 6hp
- Physical Metallurgy, 6hp
- Physics of Condensed Matter I, 6hp
- Physics of Condensed Matter II, 6hp
• 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
• Soft Condensed Matter Physics, 6 hp
• Surface Physics, 6 hp
• Thin Film Physics, 6 hp

Single subject course:
• Physics and the Environment, 6hp

Biology

STAFF

Director of studies: Agneta Johansson
Education administrator: Eva-Maria Stigsdotter
Engineers: Tove Bjerg
Teachers: Jordi Altimiras, Mats Amundin, Karl-Olof Bergman, Kjell Carlsson, Bo Ebenman, Johan Edqvist, Jenny Hagenblad, Anders Hargeby, Per Jensen, Matthias Laska, Ronny Lock, Eva Mattsson, Per Milberg, Björn Wallner, Lina Roth, Karin S Tonderski, Uno Wennergren, Dominic Wright and Thomas Östholm.

Courses in biology are offered as parts of the following study programmes:

• 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
• Chemical Biology
• Engineering Biology
• Industrial Engineering and Management
• Experimental and Medical Biosciences
• The Program for education in Linköping
• Separate courses
• Basic year

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 Programme includes, 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, and Ecology and the Environment. The profiles in Applied Ethology and Physiology are a collaboration between the department of biology at Linköping University and Kolmården’s Djurpark.

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 current program for teacher education for the Upper Secondary School and the Primary School started in 2011. The program involves a Biology and a Nature 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)
• Engineering Biology (300 credit points/hp)
• Industrial Engineering and Management (24 hp)
• Experimental and Medical biosciences (120 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 have been given.

Basic Year, with introductory courses in biology on the Upper Secondary School level.

BACHELOR PROGRAMMES
- Animal Husbandry and its Administration, 6hp
- 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, 15hp
- Ecotoxicology and Environmental Monitoring, 6 hp
- Environmental Protection and Environmental Impact Assessments, 9 hp
- Evolution 6 hp
- Genetics 6 hp
- Animal Physiology: a problem based approach, 15 hp
- Molecular Genetics, 6 hp
- Scientific Methods, Analysis and Statistics, 6 hp
- Microbiology, 6 hp
- Genes and Gene expressions, 15 hp
- Nature Conservation in Practise, 15 hp
- Principals in Physiology, 6 hp
- Zoology, Physiology, Morphology and Systematics, 6 hp

Masters of Science in Biology, profile Ecology and the Environment
- Communicating science, 6hp
- Degree Project – Master’s Thesis, 60 hp
- Methods in ecology, 15 hp
- Ecological Applications in Agriculture, Forestry and Fisheries, 9 hp
- In situ Conservation, 6 hp
- Internship in Ecology, 9 hp
- Modelling of Biological Systems, 6 hp
- Population Ecology, Theories and Applications, 9 hp

Masters of Science in Biology, profile Applied Ethology and Animal Biology
- Applied Ethology, 15hp
- Behavioral Neurobiology, 7,5 hp
- Communicating science, 6 hp
- In situ Conservation for Ethologists, 7,5 hp
- Degree Project – Master’s Thesis, 60 hp
- Methods in Applied Ethology, 7,5 hp
- Theory of Applied Ethology, 7,5 hp
- Adaptation, Genes and Molecular Evolution, 7,5 hp
- Primate Ethology, 9 hp
- Zoo Biology, 7,5 hp

Programme For Education – Biology courses
- Biology (1-15 hp), 15 hp
- Biology (16-30 hp), 15 hp
- Biology (31-37,5 hp), 7,5 hp
- Biology (38-45 hp), 1,5 hp
- Biology (46-60 hp), 15 hp
- Biology (61-75 hp), 15 hp
- Biology (76-90 hp), 15 hp
- Biology thesis, 15 hp

Engineering Biology
- Bioinformatics – Overview and Practical Applications, 6 hp
- Cell Biology, 6 hp
- Microbiology, 6 hp
- Principals of Physiology, 6 hp

Chemical Biology
- Bioinformatics, 3 hp
- Bioinformatics – Overview and Practical Applications, 6 hp
- Cell Biology 6 hp
- Genes and Gene Expression, 15 hp
- Genetics 6 hp
- Microbiology 6 hp
- Principals in Physiology, 6 hp

Chemical Biology
- Genetics and Evolution 6hp
- Bioinformatic 6hp
- Cell biology and microbial processes 6hp
- Principles in Physiology and Ethics 6hp

Separate Courses
- 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
- Senses and Behaviour of the Horse, 7,5 hp
- Ethology – Continued Course, 7,5 hp
- Faunistics & Floristics, 9 hp summer course
- Wetlands and Streams, Ecological Applications, 15 hp

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

STAFF

**Director of studies:** Magdalena Svensson  
**Education secretary:** Rita Fantl  
**Study counselor:** Helena Herbertsson  
**Technical staff:** Bo Palmquist  

**Teachers:** Anki Brorsson, Marcus Bäck, Uno Carlsson, Johan Dahlén, Karin Enander, Per Hammarström, Helena Herbertsson, Bengt-Harald Jonsson, Martin Josefsson, Peter Konradsson, Ingemar Kvarnström, Per-Olov Käll, Maria Lundquist, Patrik Lundström, Annika Niklasson, Gunilla Niklasson, Lars Göran Mårtensson, Peter Nilsson, Lars Ojamäe, Elke Schweda, Maria Sunnerhagen, Magdalena Svensson, Henrik Pedersen, Fredrik Söderlind, Gunnar Höst.

**Study programmes in Chemistry:**
- Chemistry (Ke)
- Chemical Biology (KB)
- Chemical Analysis Engineering (KA)
- 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.

All study programs consist of 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 45-120 hp of chemistry.

Besides 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** (112 students, 14 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.

In 2014 a total of 49 students graduated:
- Bachelor of Science in Engineering – Chemical Analysis Engineering (4 students)
- Bachelor of chemistry (1 students)
- Bachelor of Science Chemistry – Molecular Design/Chemical Biology (5/4 students)
- Master of Science Chemistry/Chemical Biology (2/10 students)
- Master of Science in Chemical Biology (13 students)

Altogether approximately 764 students have enrolled in about 68 courses in chemistry through the year 2014.

**NATURAL SCIENCES COURSES**  

<table>
<thead>
<tr>
<th>Course</th>
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<tr>
<td>General Chemistry 1</td>
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<td>General Chemistry</td>
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<td>General Chemistry 2</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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<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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<tr>
<td>Experimental Chemistry</td>
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<td>Physical Chemistry Spectroscopy</td>
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<tr>
<td>Analytical Chemistry - Chromatography</td>
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<tr>
<td>Organic Analytical Chemistry</td>
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<tr>
<td>Organic Synthesis</td>
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<tr>
<td>Organic Chemistry</td>
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<tr>
<td>Physical-Organic Chemistry</td>
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<td>Advanced Organic Synthesis</td>
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<td>Medicinal Natural Products</td>
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<tr>
<td>Medicinal Chemistry</td>
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<td>Molecular Design - Project Course</td>
<td>6</td>
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<tr>
<td>Protein Chemistry</td>
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<tr>
<td>Combinational Protein Engineering</td>
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<td>Biomolecular Design</td>
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<tr>
<td>Degree Project - Bachelor’s Thesis (KB)</td>
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<tr>
<td>Degree Project - Bachelor’s Thesis</td>
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<tr>
<td>Degree Project - Master’s Thesis</td>
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<td>Degree Project - Master’s Thesis (KB)</td>
<td>30</td>
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<tr>
<td>Degree Project - Master’s Thesis</td>
<td>60</td>
</tr>
</tbody>
</table>
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: Rita Fantl, Åsa Forsell, Agne Virsilaite Maras
Technical staff: Hasan Dzuho, Jonas Wissting

HIGHLIGHTS 2014

The new Basic year at LiTH started and enrolled 60 students in the first physics course.

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.
- Teacher training programmes: LÄR, ÄLP.
- Basic year and semester: BAS, BAST

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.
International Master’s Programmes

MASTER’S PROGRAMME IN APPLIED ETHOLOGY AND ANIMAL BIOLOGY

This programme 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.


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 biochemistry 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.

MASTER’S PROGRAMME IN MATERIALS SCIENCE AND NANOTECHNOLOGY

The Master’s Programme in Materials Science and Nanotechnology educates students for specialization 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 broad perspective of today’s materials science and links to applications in semiconductor technology, optoelectronics, bioengineering (biocompatibility), chemical and biosensors, and mechanical applications for high hardness and elasticity, etc.

The programme comprises four semesters. The first autumn semester dedicates mainly to the compulsory courses while the two following semesters contain a large variety of elective courses to choose among essentially four profiles.

- electronic materials and devices
- surface and nano-sciences
- theory and modeling of materials
- organic/molecular electronics and sensors

The final semester is assigned to the Master’s thesis that should be based on a high quality scientific research project within the area of the profile chosen by the student. The thesis project work can be performed either at Linköping University or at other universities.

Information about this master’s programme can be found on the web pages: http://www.liu.se/utbildning/pabyggnad/6MMSN?l=en

Progress

The programme started in 1996 with students from different countries of the world. The study results have overall been very good, and many students after graduation with an MSc degree in the areas of Materials Science continued their PhD studies at LiTH, KTH, CTH, LTH, KU, as well as at universities abroad. The programme has also been actively participating in the cooperation with other established universities in the world, such as National Tsinghua University in Taiwan, Chulalongkorn University in Thailand, Grenoble Institute of Technology in France, University of Cincinnati in USA, etc. in various ways, including double degree.
GRADUATE EDUCATION
Forum Scientium

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

Program director, director of studies: Stefan Klintström
Assistant director of studies: Charlotte Immerstrand
Chairperson of the scientific advisory committee:
Ingemar Lundström
Administrator: Anette Andersson

IFM is the host for the doctoral programme Forum 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 Fac-
ulty of Science and Engineering, three campuses; Norrköping,
US and Valla, and five departments; ITN, IKE, IMT, IFM and
IMH. Forum Scientium has financial support from the faculty
and from the supervisors.

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 2014, the doctoral programme Forum Scientium
had around 60 PhD-students, and during the year 11 PhD
and one licentiate theses were presented and 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 aims at promoting the future career for
the awardees, and to promote twinning among active Forum
Scientium members. Important is also that they should be of
benefit for the active PhD-students. The awardees are called
“Transformers” and during 2014 we had all together five
transformers.

Other activities during 2014:
• Ten monthly meetings at Campus US and Valla
• Study visit to Heidelberg/Karlsruhe/Mainz, May 2014
• Summer Conference at Båsenberga, August 2014
• Poster competition during the summer conference,
August 2014
• Yearly individual follow-up with each PhD-student
• Courses of high quality
• Life science seminars
• Together with Agora Materiae presentations of the
Nobel Prizes in Chemistry, Medicine and Physics

More information can be found at the Forum Scientium
Graduate school
Agora Materiae

AFM Director: Magnus Berggren
Graduate school head: Per Olof Holtz
Graduate school administrator: Anette Frid
Agora student council in end of 2013:
Mikhail Chubarov (Thin Film Physics, IFM)
Igor Mosyagin (Theoretical Physics, IFM)
Sit Kerdsongpanya (Thin Film Physics, IFM)
Jesper Edberg (Organic Electronics, ITN)
Lía Fernández del Río (Applied Optics, IFM)

The Agora Materiae Graduate School for PhD students working in the research field of novel functional materials was formed about three years ago, in the beginning of 2012. Today Agora Materiae has 47 members, from the three departments IFM, ITN and IEI. In year 2014, 7 PhD theses and 4 licentiate theses of Agora members were presented and defended.

Agora Materiae provides 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 Graduate School is dedicated to offer graduate studies in a true multi-disciplinary environment.

Some important activities within the Agora Materiae Graduate School during 2014:

Study visits: In May 2014, Agora Materiae Graduate School went to the company Sandvik AB for a two-day study visit. The first day, Sandvik Coromant AB in Västberga and Gimo were visited, and the second day Agora went to Sandvik Material Technology R&D in Sandviken.

Summer conference: Every year, there is a summer conference arranged during approximately three days. In Aug. 2014, the summer conference took place in Kolmården Vildmarkshotell and had this year two parts: A first part for Agora solely with invited speakers, poster presentations and outdoor activities and a second part, which was coordinated with the “mother organization” AFM for an international materials workshop with several invited speakers and researchers from industries, institutes and from universities.

Seminar activities. Every fourth week, all Agora PhD students attend seminar activities. Each time three Agora members give a presentation, and in addition one invited speaker, often a former PhD student, forward his/her experiences as a postdoc at these occasions.

Common courses. Agora Materiae graduate school arranges common courses, such as Basic Management of Research Projects and Analytical Methods in Materials Science. In year 2014, there was a new course in Presentation Techniques arranged by Agora for the first time.

Yearly individual follow-up. Each PhD student in Agora had a discussion with the graduate school director in oct/nov 2014 to discuss project, progress, time schedule, but also problems in the graduate program.

Nobel lecture. Prof emeritus Bo Monemar from IFM lectured on Nov 26 about the Nobel prize 2014: “The invention of efficient blue light-emitting diodes which has enabled bright and energy-saving white light sources”. Prof Monemar has been collaborating with two of the Nobel prize winners for more than 20 years, and was awarded as Honorary Doctor at Nagoya University in October 2006. Prof Monemar has been working as a visiting researcher in Japan during the autumn 2014.
IFM Graduate Programme

Director of graduate studies: Per Olof Holtz

The graduate program at IFM aims at a degree of Licentiate or Doctor of either Technology or Philosophy. During the year 2014, 26 new PhD students entered the graduate program at IFM (see diagram below). In order to get a PhD or a licentiate exam, the student will partly complete a number of graduate courses and partly perform research work resulting in a doctoral/licentiate thesis. The nominal time for training to the Doctor degree is four years with full-time training, while the corresponding time for the Licentiate degree is two years. However, most students also do teaching at undergraduate level (up to 20% of their time) or alternative duties, which means that the total time to provide the Doctor degree can be up to five years, or 2.5 years for the licentiate degree. The graduate students at IFM do, at an average, teaching at 10% of their time.

Diagram I showing the number of students entering the graduate program at IFM during the last four years.

At IFM, the required number of credit points for a PhD / Licentiate exam, varies in the range 60-90/30-45 hp for the different research areas. For the course work required for the respective exam, there is an extensive course menu offered for the IFM PhD students. The course menu is organized jointly by the different scientific research groups. During the academic year 2013/14, the PhD students could choose among about 60 courses at IFM.

The students are also offered to follow courses arranged by the technical faculty, which are of a more general character, such as entrepreneurship, IPR and writing scientific papers. The students can also follow courses given at the graduate schools Forum Scientium and Agora Materiae at IFM, at other departments of Linköping University or at other universities.

There are three mandatory courses for all PhD students: i) Research Ethics, 2 ECTS, ii) Methodology of Science and Technology, 4 ECTS and a course in teaching in higher education of at least 3 ECTS (the course is mandatory for all PhD students that have teaching duties).

At IFM, a specific pedagogic course is arranged, including e.g. content-specific challenges and how to assist students in a laboratory environment. The course consists of four blocks and an introductory meeting, seminars, lectures and auscultation following an experienced university teacher.

At IFM, there is a Board of Graduate Education, which 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.

Each new PhD student at IFM will get a mentor. There are several reasons for the mentorship system at IFM, e.g. that each PhD student should have the possibility to go to another person than his/her supervisor with various questions related to the graduate studies. This system should open up the possibility for the PhD students to discuss problems associated with the PhD program with the mentor. The mentor is also taking part in the annual follow-up of the individual study plans.

IFM is the base for two graduate schools: Agora Materiae within the area of material science and Forum Scientium with its focus towards life science. These graduate schools also attract PhD students from other departments (e.g. ITN and IEI) within the technical faculty, but also from the medical faculty (HU).
General Information

STEERING COMMITTEE DURING YEAR 2014

Comprises the heads of divisions: Prof Mats Fahlman, prof Anita Lloyd Spetz, prof Kajsa Uvdal, assoc prof Thomas Ederth, prof Kenneth Järrendahl, prof Olle Inganäs, prof Carl-Fredrik Mandenius, prof Anthony Turner and ass prof Stefan Klintström (chairperson).

RESEARCH DIVISIONS AND PROFESSORS

Applied Optics: Kenneth Järrendahl (Head of division), Hans Arwin

Applied Sensor Science: Anita Lloyd Spetz (Head of division)

Biomolecular and Organic Electronics: Olle Inganäs (Head of division), Fengling Zhang

Biosensors and Bioelectronics: Anthony Turner (Head of division) Fredrik Winquist, Ingemar Lundström (Emeritus)

Biotechnology: Carl Fredrik Mandenius (Head of division), Anders Brundin (Adjunct)

Chemical and Optical Sensor Systems: Ragnar Erlandsson, Helen Dannetun (Rector Linköping University), ass prof Stefan Klintström (Head of division)

Complex Materials and Devices: Martijn Kemerink

Molecular Physics: Bo Liedberg, assoc prof Thomas Ederth (Head of division, assoc prof Daniel Aili (Assistant head of division)

Molecular Surface Physics and Nanoscience: Kajsa Uvdal (Head of division)

Surface Physics and Chemistry: Mats Fahlman (Head of division), assoc prof Nathaniel Robinson (Assistant head of division)

LARGER RESEARCH PROGRAMMES

• Strategic Faculty Grant AFM – Advanced Functional Materials
• Strategic Faculty Grant Security Link
• VINNOVA Challenge driven innovation (UDI) project Online sensor system for resource-efficient water management (Sensation)
• VINNOVA VINN Excellence Centre FunMat
• Linköping Initiative for Life Science Technologies (LIST)
• The Linköping Center for Nanoscience and Nanotechnology – CeNano
• “Power Papers” funded by the Knut and Alice Wallenberg foundation
• “Designed Nanoparticles by Pulsed Plasma” funded by the Knut and Alice Wallenberg foundation
• “Working on Venus” (WOV) funded by the Knut and Alice Wallenberg foundation

INTRODUCTION

The research within the Scientific Branch of Applied Physics spans over a large scientific area, e.g. surface and molecular science, biotechnology, lab-on-a-chip, nanoscience, organic electronics, optics, bio- and chemical sensors.

During 2014, we had 44 PhD students within the Scientific Area Applied Physics.


In addition, one PhD student presented her Licentiate: Alina Sekretaryova (Chemical and Optical Sensor Systems)

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

HIGHLIGHTS DURING 2014

Applied Sensor Science

Sensors based on epitaxial graphene on silicon carbide (grown by IFM/ MS, Rositsa Yakimova) have been decorated by nanoparticles, deposited by Plasma & Coatings Physics (Ulf Helmersson). While the graphene properties were retained, sensors decorated with TiO2 nanoparticles responded to ultra-low concentrations of formaldehyde and benzene (toxic substances at ultra-low levels, to which pristine graphene sensors do not respond), where the nanoparticle size determines the selectivity.

JF Prize 2014

Anita Lloyd Spetz was awarded the JF Prize 2014 during the LiU Junior Faculty Career Day, held in Planck on 14th November. The JF Prize is assigned every year to a senior researcher from Linköping University for his/her outstanding merits in supporting and encouraging young researchers to build their own successful professional career.

JF Prize designed by Chil Loong, Concept Cove shop, Gamla Linköping
Biomolecular and Organic Electronics

organized and participated in the 1st Ethio-Swedish workshop on organic photovoltaic materials and wooden batteries in Addis Abeba, Ethiopia, November 27-28, 2014. We celebrated more than 20 years of collaborations with the goal of establishing an independent research capacity in the field of organic materials for energy conversion and storage. This goal is now accomplished.

World’s Most Influential Scientific Minds

Prof. Olle Inganäs and Prof. Fengling Zhang were both awarded the “World’s Most Influential Scientific Minds” http://highlycited.com/ award by Thomson Reuters.

Surface Physics and Chemistry – Organic Physics Group

have developed a general model treating the effects of doping and intermolecular order on energy level alignment at organic and hybrid organic heterojunctions, while also demonstrating new design rules for minimizing open circuit loss in organic bulk heterojunction solar cells.

Surface Physics and Chemistry – Transport and Separations Group

has continued its progress in developing “soft” (e.g. polymer) electronic systems for chemistry and biology applications, including projects demonstrating the use of 3D printers to fabricate microfluidic systems.

Top Position for Biosensors & Bioelectronics Journal

The Impact Factor of our journal Biosensors and Bioelectronics (Elsevier), edited at IFM by Alice Tang-Turner, Tony Turner and Ingemar Lundström, has leapt from 5.4 last year to an all-time high of 6.5 for the current year. This places it in first position for research journals in the entire field of Analytical Chemistry.

Integated Biosensor Platform Demonstrated at Biosensors 2014

At the World Congress on Biosensors LiU had an exhibition stand together with Acreo Swedish ICT AB, where we demonstrated, for the first time, the Integrated Biosensor Platform resulting from a joint R&D programme between the Biosensors and Bioelectronics Centre and Acreo Swedish ICT AB. By combining the virtues of printed biosensors and organic electronics, we have introduced a new disposable instrument range exploiting the latest advances in printed electronics.

Chemical Sensor Systems

developed for field measurements have during 2014 been successfully tested at the lake Mälaren. One system is based on the electronic nose technique and is an early warning sensor for petroleum contamination. It has a detection limit below the required 5 ppb for diesel. The other system is based on the electronic tongue technique and is an early warning sensor in general and for sewage water, a marker for pathogenic micro-organisms, in particular.
We combine material optics and development of ellipsometric methodology to analyze optical properties and nanostructure of bulk materials, thin films and their interfaces.

Our main technique is spectroscopic ellipsometry which is based on analysis of changes in the state of polarization of light interacting with matter. Our instruments cover the spectral range 0.19–33 micro m (0.04–6.5 eV) and provide generalized ellipsometric data as well as depolarization and Mueller-matrix data. Our software allows analysis of the dielectric $\varepsilon$, magnetic $\mu$ and gyrotropic $\xi$ and $\zeta$ tensors at optical frequencies. Using these features we can address materials properties of nanostructured materials in the emerging field of metamaterials.

Optical properties of cuticles of several species of beetles found primarily in Europe and South America were studied to learn how nature has designed biomultilayers. Of special interest is to understand the polarization properties of light reflected and/or scattered from cuticles as well as relation between optical properties and structure. For Cetonia aurata, Mueller matrices have been analyzed and in collaboration with Ecole Polytechnique in Paris we have explored decomposition of Mueller-matrices as a mean to characterize and classify cuticles. Optical modes in the cuticle of Cotinis mutabilis were studied. From interference oscillations in Mueller matrix elements, a dispersion relation similar to that of optical modes in nematic liquid crystals were studied. A structural model for the cuticle was derived from the properties of these optical modes (see figure below). Light and electron microscopy were used as complementary techniques to resolve structure and understand scattering properties. Spectroscopic ellipsometry was used to study the optical properties as well as changes induced in amorphous and semi-crystalline chitin thin films by humidity and temperature. Chitin is a semi-crystalline biopolymer found in the cuticles of beetle as nanofibrils in a helical lamella structure which is responsible for the fascinating and complex polarization properties. As a complement to our chitin studies we have in collaboration with researchers in Mexico fabricated and analyzed transmission properties of free-standing chiral cellulose films. To further understand cuticle structure we have also initiated ellipsometric transmission measurements on beetle cuticles. (Arwin, Berlind, Fernández, Hallberg, Järrendahl, Landin, Magnusson, Muñoz, Mendoza, Valyukh, Åkerlind).

The Polarizance vector $[m_{21}, m_{31}, m_{41}]^T$ at a fixed incident angle of 25° of a left-handed chiral InAlN film.
LIQUID CRYSTAL BASED OPTICAL ELEMENTS

Lenses with variable focal distance, switchable phase arrays and beam steering devices based on liquid crystals were studied. The main focus was on development of non-uniform alignment conditions that enable us to achieve the needed distribution of the liquid crystal molecules under a uniform external electric field.

An objective LC micro-lens array for displays located at the immediate vicinity of the eye, e.g. in contact lenses or glasses, has been proposed. This work has been made in cooperation with H. De Smet and co workers (Ghent University) who has fabricated a prototype of such a display. The developed objective LC micro-lens array changes optical power from 0 to up to 5000 dioptres that makes it possible to see the display image and the surroundings clearly, i.e. confers the ability of augmented reality. (S. Valyukh).

SCIENTIFIC OUTPUT 2014


SPECIAL EVENT

Roger Magnusson defended his PhD. thesis on December 12, 2014.

TEACHING

Järrendahl, S. Valyukh and Arwin were responsible/examiners for many optics related undergraduate courses and activities. Fernández del Río, Magnusson and I. Valyukh was involved in several courses during the year. Järrendahl was vice chairman for the EF study board.

Applied Sensor Science

STAFF

Professors: Anita Lloyd Spetz
Associate professors: Dr Mike Andersson
Assistant professor: Dr Robert Bjorklund (retired Oct 2014), Dr Jens Eriksson, Dr Donatella Puglisi
Post Doc: Zhafira Darmastuti (from July 2014)
Administrative staff: Therese Dannetun
Graduate students: Zhafira Darmastuti (PhD exam June 2014), Christian Bur, Hossein Fashandi, Peter Möller, Lida Khajavizadeh (from Oct 2014)
Research engineers: Peter Möller

RESEARCH ACTIVITY

Division of Applied Sensor Science participates in The Vinn Excellence Center FunMat (Lloyd Spetz Centre Head), Advanced Functional Materials, AFM, and run projects together with the Divisions of Material Science and Plasma & Coating Physics.

Lloyd Spetz holds a FiDiPro, Finland Distinguished Professor, at University of Oulu, 50%, 2011-2015. The research project concerns development of a portable nanoparticle detector and a device for detection of toxic effect of particles on cells. From March 2013, Docent Mike Andersson has 25% position at University of Oulu.

We participate in the COST Network, EuNetAir TD1105 (Lloyd Spetz Deputy Chair), New Sensing Technologies for Air-Pollution Control and Environmental Sustainability (partners from 36 countries).

THE JUNIOR FACULTY PRIZE 2014

Professor Anita Lloyd Spetz was awarded the Junior Faculty prize 2014 for supporting and encouraging young researchers to build their own successful professional career.

NEW GENERATION SiC-FET GAS SENSORS

The SiC-FET gas sensors developed by the spin-off company SenSiC AB in collaboration with Applied Sensor Science and FunMat, could be hermetically included in the LTCC, Low temperature co-fired ceramic, packaging during processing. This is a collaboration with University of Oulu, Finland. The LTCC technology provides possibility to integrate smart functionality in the packaging.
**PARTICLE DETECTION**

Ammonia containing ash particles were heated to 430°C and the release of ammonia detected by SiC-FET devices. Heating particles and detecting the emissions by gas sensors may give a fingerprint of the content/adsorbents of the particles. This is a collaboration with Saarland University, Saarbrücken, Germany, and University of Oulu.

**GRAPHENE SENSORS**

Monolayer graphene, epitaxially grown on SiC in the group of Prof Rositza Yakimova, IFM/ MS was characterized for gas sensing and shows ultra-low detection limit, less than 10 ppb of NO₂. Decoration by metal or metal oxide nanoparticles (e.g. TiO₂) through plasma deposition processing in the group of Prof Ulf Helmersson (grant from CeNano) enabled ultra-low detection limits of formaldehyde and benzene. Particle size contributes to selectivity.

**MONOLAYERS FOR SENSING**

A monolayer of iron oxide on top of porous Pt in a silicon carbide- silicon dioxide capacitor showed an increased catalytic activity to the CO to CO₂ oxidation reaction. The CO gas sensing showed an optimum at about 40°C lower temperature due to the monolayer of iron oxide, processed at KTH, Stockholm. The monolayer iron oxide-Pt sensor was stable during 200 hours of operation.

**SMART SENSING**

In collaboration with Prof. Andreas Schütze, Saarland University, smart sensor operation of SiC-FETs and advanced data evaluation are developed. Cycling of the operation temperature and applied gate bias together with smart data evaluation improves largely the information from SiC sensors. Quantification of NO and NO₂ in a (varying) mixture of synthetic exhaust is demonstrated. Christian Bur is PhD student in the project at both Saarland and Linköping Universities within the research school DocMASE.

**VOC DETECTION DOWN TO SUB-PPB LEVELS**

Catalytic metal-gated SiC-FETs were investigated in up to 60% relative humidity (r.h.), demonstrating high, stable, and reproducible performance. Detection limits of 10 ppb for formaldehyde, 1 ppb for benzene, and below 0.5 ppb for naphthalene at 60% r.h. were determined. These results are very encouraging for indoor air quality control, being below the threshold limits of EU and US legal requirements.

**SENSING ON VENUS**

In the KAW project, Working on Venus, coordinated by KTH, Stockholm, we develop electronics and sensors for the environment on Venus. This implies a temperature of 460°C in an atmosphere of 96% CO₂, 3.5% N₂, 0.5% H₂O and trace amounts of H₂SO₄, HCl and HF at a pressure of 92 bar! While silicon based electronics only functioned for a short time in this atmosphere, SiC is potentially a suitable material for electronics and sensors in this environment.

![3-D radar image of the Maat Mons volcano on Venus](image)

**NOₓ SENSING**

SenSiC AB is coordinating a FFI-project (Fordonsstrategisk Forskning och Innovation) where Applied Sensor Science and Chalmers together with industrial partners VOLVO AB and SCANIA develop a NOₓ sensor for after treatment of diesel engine exhausts.

**SO₂ SENSING**

In a FunMat project with Alstom Power Sweden AB in Växjö we have developed SO₂ sensors for control of the desulphurization unit in power plants. The SiC-FET sensors could detect the interesting sulphur concentration when operated in a temperature-cycled fashion. Zhafrica Darmastuti defended her PhD thesis in this project in June.
A SiC-FET follows the SO$_2$ concentration in a small heating plant. [Darmastuti et al, Sensors and Actuators B, 206 (2015) 609-616]

**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) on MAX materials (conducting ceramics) for ohmic contacts to SiC, new sensing layers for SO$_2$, H$_2$S, NO/NO$_2$, O$_2$ and PM sensor for diesel exhausts.

**Biomolecular and Organic Electronics**

**STAFF**

*Professor*: Olle Inganäs, Fengling Zhang

*Associate professor*: docent Niclas Solin

*Visiting scientists*: Shimelis Admassie (April–Sept).

*Postdocs*: Feng Gao, Mingtao Lu, Ting Yang-Nilsson, Michal Wagner, Chiara Musumeci (May–), Wanzhu Cai (Sept–), Lianggui Ouyang (Oct–), Bo Liu (Oct–), Mikhail Vagin (70%)

*Graduate students*: Anders Elfving, Fredrik Bäklund, Zheng Täng, Jonas Bergqvist, Armantas Melianas, Erica Zeglio, Fatima Aijan, Deping Qian, Yuxian Xia, Daojung Wang

*Research assistants*: Sophie Kaldlin (March–), Patrik Johansson (June–September), Anjula Ratnayake (Aug–)

*Visiting students*: Yuxian Xia (Jan–Sept), Rosanna Mastria, Anna Maria Uhlin

*Research engineer*: Bo Thunér (27%), Mattias Andersson

*Diploma students*: Sofie Kaldlin, Olof Andersson, Josef Lautin

**SUMMARY**

Research in biomolecular and organic electronics is focused on the development of organic electronics, particularly organic photovoltaics, and the combination of biological macromolecules with synthetic conjugated polymers for supramolecular materials assembly. We published 33 papers during 2014.

**BIOMOLECULAR ELECTRONICS**

We develop biopolymer based polymer electrodes, where an electronic polymer is storing charge in a modified biopolymer carrying quinone groups. We have developed modified lignins for improved charge capacity. A new conjugated polymer has been found, where quinones are part of the backbone, and where the severe problem of self-discharge found with polypyrrole based electrodes is suppressed. We find out that with these type of materials there is a possibility to attain over 200 mAh/g of charge capacity and over 1000 F/g of capacitance at discharge currents of 1 A/g. These polymer electrodes are of relevance for energy storage in supercapacitors and secondary batteries based on aqueous electrolytes.

Another possibility is the design of these materials for extraction of heavy metal ions out of water. We have developed a biopolymer electrode where the metal ion sorption is high, due to coordination to quinone groups within the material. The metal ion is adsorbed at one potential, and released at another potential. Such electrodes play the double role of cleaning water from lead, as well as storing charge from photovoltaic modules at day, to be released during discharge at night, thus helping to improve both electricity and water supply.

We demonstrated how the metallic polymer PEDOT-S can integrate into bilayer lipid membranes, forming an electronically conducting element inside a liposome. We have used such liposomes to modify egg cells from frog, and can show
that the ion conductance characteristics of the ion channels inserted in the frog cell are modified.

Materials containing cavities and pores are desirable. Amyloid fibrils are such a material as the assembly of β-strands leads to the formation of ordered patterns of ridges and grooves. These structural elements have dimensions suitable for binding of flat π-conjugated molecules. We have utilized these features of amyloid fibrils to disperse and organize various hydrophobic π-conjugated molecules, including laser dyes. This opens up the possibility of utilizing amyloid fibrils as a solid state matrix pre-patterned for inclusion of luminescent dopants.

We have prepared materials where amyloid fibrils are used as templates for organization of conjugated polymers such as PEDOT-S. The methodology has been extended to include hierarchically assembled amyloid fibrils – resulting in chiral protein superstructures – that can transfer optical activity from the protein structure to the achiral conjugated polymer.

**ORGANIC PHOTOVOLTAICS**

New materials are continuously demonstrated in organic photovoltaic devices, with most polymers synthesized at Chalmers University. Our present high polymer/fullerene performers deliver power conversion efficiency ≈ 8%. Ongoing studies of transient energy and charge flow through these structures strongly emphasizes the fact that these devices do not operate under thermodynamic equilibrium conditions, and that non-equilibrium sets very important conditions for collecting the photogenerated current.

To increase photocurrent, the absorption spectrum of absorbers must overlap with the solar spectrum. A series of low band-gap molecules with absorption to 800 nm gave power conversion efficiency up to 5.0%.

A new approach is the combination of donor molecules and polymeric n-type acceptors, which can be blended to make well performing materials. The very low driving force for charge transfer in such blends still allows an efficient formation of charge carriers. In polymer/polymer blends, where efficiencies of 4% have now been reached, great opportunities exist for improved optical absorption.

We have demonstrated the use of semitransparent metallic polymer electrodes in organic solar cells, with modifications of one of these layers to make it operate as a cathode. Semitransparent solar cells on flexible foil is the target for our project on printing of solar cells using roll-to-roll methods at high speed. We have now upscaled the synthesis and printing of materials for semitransparent OPV.

We demonstrated a dual functional EC/PV window type device, a solar-powered electrochromic (EC) smart window switched between transparent and colored states for modulating incoming solar irradiation, to decrease electricity consumption for air conditioning and with PV panel for converting sunlight into electricity. The EC/PV windows will be very useful for passive houses and urban skyscrapers.

We organized the 1st Ethio-Swedish workshop on OPV and wooden batteries in Addis Abeba, Ethiopia, November 27-28, 2014.

**PHD DISSERTATION**


**TEACHING**

Teaching in the undergraduate curriculum included:

CDIO project for Engineering Physics (Building a solar simulator from scratch). Microsystems and nanobiology (TB), Materials and nanotechnology (TB), Introduction to renewable energy and energy saving (Y). Condensed soft matter physics


The Wallenberg Scholar fund for Olle Inganäs has been instrumental in creating novelty.

**HIGHLIGHTS**

Semitransparent solar cells on a light powered electrochromic window.
Biosensors and Bioelectronics

STAFF

Professors: Anthony (Tony) Turner and Fredrik Winquist
Emeritus professor: Ingemar Lundström
Associate professors: Valerio Beni, Edwin Jager, Martin Wing Cheung Mak, Ashutosh Tiwari and Lokman Uzun
Managing editor: Dr Alice Tang-Turner
Visiting scientists: Anis Nurashikin Nordin
PhD students: Mohsen Golabi, Onur Parlak, Alina Sekretaryova
Visiting PhD students: Amir Hatamie, Usisipho Feleni, Ceasar Hernandez, Roghayeh Imani, Kamalodin Kor, Yu Liu, Erdogan Özgur, Elham Sheikzadeh and Mykhailo Zhybak.
Master students enrolled at LiU: Katarina Eken, Erika Johansson, Sureesh Kollipara, Marjam Memarpuri and Hama Nadhom.
Research Administrator: Anette Andersson

GENERAL INFORMATION

The division averaged a compliment of ~30 researchers in 2014. We published 34 journal papers, 20 conference papers, 2 book chapters and 6 books in 2014 (DIVA). The Centre’s overall mission remains the creation of next generation bioelectronic devices with a focus on distributed diagnostics for health and the environment. Key strategic targets include fully-printed electrochemical sensing systems, optical biosensors, wearable sensors, mobile health, lateral-flow devices and the creation of new biomaterials and smart tissue scaffolds: www.ifm.liu.se/biosensors

HIGHLIGHTS

Integrated Biosensor Platform

Joint programme with Acreo Swedish ICT AB. Mobile diagnostics for healthcare, food safety and environmental monitoring demand a new generation of inexpensive sensing systems that can be produced in high volume, to open up new market niches. By combining the virtues of printed biosensors and printed electronics, we have introduced a new disposable instrument range. This approach combines the sophistication of advanced electrochemical biosensors with a simple manufacturing technique to create a use-and-throw instrument. Initial proof-of-principle was achieved for the detection of glucose and this is now being expanded, with the help of LiU diploma students Katarina Eken and Erika Johansson, to include enzyme electrodes for lactate and β-hydroxybutyrate, all of which are key in the management of diabetes.

Dengue Screen: Point-of-care µTAS for sensitive and rapid detection of dengue

Swedish Research Council – VR International collaboration grant – VR (2015-2018), 675k SEK. This bilateral collaboration between Martin Mak (LiU) and Dr. Nordin (International Islamic University, Malaysia) is to develop a new biosensor for dengue virus for cost effective management of dengue in low and middle income countries, where access to resources is limited. The latest figures from the Malaysia health authority show a dramatic four-fold increase in dengue cases reported accompanied by a three-fold increase in the number of deaths in the first quarter of 2014. This is a global threat affecting not only local citizens, but also billions of international travelers. The Dengue-Screen project strengthens the established collaboration between our two universities and facilitates future funding.

Biosensors to monitor multiple metabolites for sensitive, reliable and personalised management of diabetes

LIST (2014-2015), 200k SEK. Martin Mak and Tony Turner received this grant to develop cost-effective, printed biosensors to monitor multiple metabolites for sensitive and reliable management of diabetes. This project aims to monitor multiple metabolites simultaneously and use cloud-based expert systems to improve management.
**Biosensors for chronic kidney disease**

IF Sensing Ltd. Phase 1: 845k SEK, 2014. A six month feasibility study was carried out by Tony Turner, Martin Mak and Valerio Beni for IF-Sensing Ltd. (UK), which was funded by the UK Technology Strategy Board to investigate novel biosensors for the detection and management of chronic kidney disease. The study delivered a working prototype for one key analyte. This provided the basis for a successful application for Phase II funding from the UK Government and an expanded programme will commence in 2015.

**Detecting bioluminescence with organic photodetectors for biosensing of colon cancer**

LIST (2014-2015), 200k SEK. This collaboration between Drs. Mak, Zhang and Sun aims to use organic photodetectors (OPDs) as miniaturised cost-effective bioluminescence transducers in biosensors to monitor gene expression in colon cancer cells. Bioluminescence has been widely used for applications such as measuring adenosine triphosphate, and studying gene expression and cellular events coupled to gene expression. Current technology is based on bulky equipment and time-consuming procedures. Our goal is to develop biosensing tools to help elucidate the mechanism of colon cancer and improved therapies.

**Lateral-flow tests for rapid, cost effective and sensitive detection of micro-RNA**

Martin Mak and Valerio Beni initiated this project for Kamalodin Kor (Damghan University, Iran). Micro-RNAs (miRNAs) are a class of noncoding RNA molecules, between 17 and 25 nucleotides long, encoded in the genomes of plants and animals. miRNAs are involved in e.g. early development, cell proliferation, cell apoptosis, fat metabolism and cell differentiation. We developed a lateral-flow strip test for simple, rapid and specific detection of miRNA-21 based on a generic single-probe assay using structurally responsive biotin-oligonucleotide-AuNPs biolabels. The test is linear over the range 0.5 to 20 nM miRNA with a cut-off detection limit of 0.5 nM, and has high specificity over other miRNAs. The test was demonstrated in spiked serum samples.

**Molecularly Imprinted Nanofibres for Tissue Engineering, Affinity Depletion and Biosensor Applications “MIFs4BioMed”**

Marie Curie IEF (2014-2016), 2.6m SEK. The design and synthesis of biomimetic functional polymers, using polymerisable derivatives of biomolecules for molecular imprinting, offers exciting potential advantages over conventional biomaterials with respect to reusability, stability, shelf-life, chemical and physical resistance, and ease of preparation. In our initial work, we have created molecularly imprinted hydrogels for protein chromatography as a tool for isolating interfering molecules.

**High-throughput electrocatalytic nanobioreactors**

We have fabricated a novel two-dimensional nanobioreactor, consisting of gold nanoparticle-structured tungsten disulphide nanosheets, which offers a simple and effective way to overcome many previous limitations and has applications in bioreactors, biofuel cells and biosensors.

**Registration of nanoparticle-microelectrode collisions:**

CeNano (2014-15), 75k SEK. Martin Mak and Mikhail Vagin are developing a new platform for nanoparticle (NP) characterisation, which will explore the electrochemical behaviour of nanoparticles and their application, thus enhancing two ongoing PhD projects: Alina Sekretaryova (electrochemical detection of nanoparticles) and Onur Parlak (nanomaterial biosensors).
Cell microencapsulation and monitoring: a step towards cell therapy

Delivery of stem cells to achieve tissue regeneration is challenging. Microencapsulation provides a new strategy by creating a semi-permeable container between the encapsulated cells and the environment, which may improve the efficiency of cell delivery to the target tissue. In parallel, monitoring of the encapsulated cells inside the microcapsule environment is important to optimise the microcapsule construct design and therapeutic efficacy. LiU Master student, Diana Atanasova, and a new PhD student, Kim Olesen, are jointly supervised by May Griffith (IGEN) and Martin Mak to develop an encapsulation technique based on hydrogels and to monitor cells within microcapsules. The initial focus is on controlling and monitoring the proliferation of MSC cells within microcapsules and then testing in animal models as a cardiac patch for heart muscle regeneration.

Smart cancer nanotheranostics

We are seeking to integrate therapeutic and diagnostic platforms to combine real-time monitoring with drug delivery. Initial evaluations of our material have indicated its suitability for smart cancer theranostics.

Smartcancersens, PiresesGA-2012–318053

Under this continuing 4-year EU IRSES programme, the Centre hosted two more PhD students. Mykhailo Zhybak (National Academy of Sciences of Ukraine) continued his work on the development of chemi/biosensors based on novel Cu/Nafion/PANI nanocomposites. Usisipho Feleni (University of the Western Cape, South Africa) came to work on electrochemical biosensors exploiting Cytochrome P450, in conjunction with quantum dots, for very sensitive detection of Tamoxifen. The development of such a biosensor is of great importance in improving breast cancer treatment by optimising the effective dose of the drug and reducing its side effects.

Polypyrrole-based biosensors

Valerio Beni and Edwin Jager continued to explore the use of polypyrrole for the development of novel chemi/biosensors. As part of her master thesis, Laurence Padiolleau developed a highly specific chemical sensor for dopamine based on over-oxidised polypyrrole doped with a specific ligand. Mohsen Golabi and Elham Sheikhzadeh investigated the use of functional dopants and/or modified pyrrole monomers for modulating the adhesion of bacteria onto surfaces and for the development of bacteria biosensors, following functionalisation of the polypyrrole film with aptamers.

Pathoscreen, VR international cooperation grant (650k SEK), 2014–2016. In collaboration with the Istanbul Kemerburgaz University (Turkey), we are developing electrochemical aptamer-based biosensors for the detection of pathogens (i.e. S. typhimurium and E. coli) in food/environmental samples. Valerio Beni and visiting student, C. Hernandez (Universidad de los Andes, Colombia), explored different strategies for the integration of aptamers and screen-printed electrodes. As part of the same project, Mohsen Golabi visited Istanbul to perform the selection of novel multiple-target aptamers based on a new concept of cell SELEX.

Smart scaffolds for cardiac regeneration

IGEN (2012–2014) 800k SEK. Engineered smart scaffolds are an interesting alternative to deliver stem cells. We are developing smart scaffolds for cardiac regeneration and improved stem cell differentiation. Employing a novel synthesis protocol developed by IGEN-fellow Amy Gelmi, we can reproducibly produce electroactive scaffolds that are biocompatible with a variety of cells, including cardiac progenitor cells and induced pluripotent stem cells. In collaboration with Marek Los and Artur Cieslar-Pobuda (HU), we are currently investigating the effects of electro-mechanical stimulation on stem cell differentiation into cardio-myocytes.
We also received a large collaborative VR MH grant with Dr Karl Svennersten and Dr Katarina Hallén Gruftman, MD, at the Karolinska Institute as co-applicants. In this project we will study mechanotransduction in the urinary tract using our unique mechanostimulation chip-technology.

**Polymer actuators**

**COST Action MP1003 (2010-2014); Carl Trygger Foundation (2013-2015) 535k SEK.** We continue our development of new actuator hybrid materials comprising carbide derived carbon as well as new actuator geometries. Our Carl Trygger project received a second-year extension with Ali Maziz continuing the work of Janno Torop.

This was also the final year of the COST action MP1003 “ESNAM”. We received three guest researchers, Adelyne Fannir, Dr Ali Maziz and Dr Ingrid Graz, through the COST exchange program, working on different polymer actuator designs and new materials. Alexandre Khaldi presented the successful LIU COST collaborations at the Final Event 25-26 Nov 2014, in London.

**Power-on-demand biofuel cells**

Our recent research on enzymatic biofuel cells has focused on increasing the life-time and energy density via enzyme cascades to increase the degree of oxidation of the fuel, improved electron transfer pathways and novel immobilisation techniques. We are now focusing on incorporating functional materials at the electrode surface to deliver power-on-demand biofuel cells with tunable output, using high-permeability ion-conducting nano-frameworks.

**Soft Microrobotics**

**POLYACT Marie Curie Fellowship (2014–2016) 198k EUR.** We are developing soft microrobotics based on conducting polymer actuators for biomedicine. Marie Curie Fellow, Alexandre Khaldi, has progressed the microfabrication of polymer trilayer actuators that can operate in air and can be individually addressed. Detailed characterisation of the new devices is on-going. Edwin Jager’s collaboration with the University of Wollongong (Australia) continues through his visiting senior scientist position and this project. During a visit in May 2014, we progressed novel patterning methods of conducting polymer actuators.

A PPy trilayer actuator unit with two individual controllable microfabricated actuators.

**Marie Sklodowska Curie Action Innovative Training Network**

**MICACT (2015-2018) 527k EUR.** As a spin-off from the COST action MP1003 we were able to secure a MSCA Innovative Training Network in the area of electroactive polymer micro-actuators. LiU will host 2 PhD student positions. The students will be recruited during the spring 2015.

**TEACHING**

LBB strengthened its position in education at LiU giving and/or designing a series of courses, based on both theoretical and practical classes. The Centre runs key courses in the area of biosensors including: Introduction to Biosensor Technology (TFYA62), for 2nd year students of the Biomedical Engineering bachelor degree, and Biosensor Technology (TFTB34). The Centre also continued teaching at PhD level. Valerio Beni and Mikhail Vagin designed and ran a new course in Applied Electrochemistry and Ashutosh Tiwari delivered two courses: Bioengineered Nanomaterials and Smart Materials and Methods. Five more LiU students completed their Diplomas with us along with 8 visiting Masters’ students. Our team also delivered a number of other lectures on other courses and received excellent feedback. Edwin Jager and Martin Mak hosted group projects for CDIO courses: “Medicinsk Teknik” TBMT41 and “ingenjörsprojekt” TFYY31.
Biotechnology

STAFF
Professors: Carl-Fredrik Mandenius (Head of division), Johan Hyllner (Adjunct), Gunnar Hörnsten (Adjunct)
Associate professor: Danny van Noort
Research engineer/Lab manager: Robert Gustavsson
PhD candidates: Gunnar Bergström, Inga Gerlach, Jonas Cristoffersson, Robert Gustavsson
Project workers: Alexander Reissig, Micael Karlberg
Administration: Susanne Andersson

SUMMARY
The Division of Biotechnology research in engineering biology and teach with focus on industrial biotechnology. Research projects encompass applications of monitoring, modelling and control of bioprocesses, in vitro bioanalytics for drug testing and conceptual design methodology for biotechnological products.

The division is active in the LiTH programmes Engineering Biology and Chemical Biology by providing courses in Industrial Biotechnology, Bioproduct Design, Biomanufacturing and supervising master projects in biotechnology.

The PhD-study program in biotechnology provided by the Division connects to the topics and is by that an important part of the research. Moreover, the integration of the topics in the curricula of the Engineering Biology program forms an important link between education and research at the Division.

HIGHLIGHTS

EU-project StemBANCC
In StemBANCC (www.stembancc.org), an IMI-EU project with 40 partners from the European pharmaceutical industry and academia, we tailor Lab-on-a-Chip devices for the monitoring of patient-specific cells derived from induced pluripotent stem cells.

In the project 600 induced pluripotent stem (iPS) cell lines are used to study a range of diseases, including diabetes and dementia, in particular efficacy and safety of new drugs under development. 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. Lab-on-a-Chip assays are one of the key methods applied in the project.

Lab-on-a-Chip for reducing animal experiments
In another related project we investigate together with the group of Dr Nate Robinson at IFM other Lab-on-a-Chip design concepts for toxicity assaying aiming at reducing animal testing.

In parallel we develop other applications of microfluidic devices in combination with high-sensitive fluorescence detection (Fritzsche et al, 2014).

Lab-on-a-Chip device for monitoring of liver cells (Fritzsche et al, 2014).

Soft sensors for bioprocess monitoring and control
Soft sensors are robust on-line sensors supported by mathematical models derived from the bioprocess systems to be monitored and controlled. The soft sensors are useful for bioprocess monitoring due to the complexity of the biological mechanisms of the producing cells. We use different soft sensor architectures 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, J Chem Technol Biotechnology, 2015).

During 2014 a soft sensor study on using heat balances for estimation of specific growth rate has been performed (Paulsson et al, 2014).

During 2014 have also two master thesis projects been carried out where soft sensors using thermometric and capacitive sensors are applied to mammalian cell cultures.

Principle of a soft sensor for bioprocess control

EU-project BIORAPID
A new EU Marie Curie project (ITN) on accelerating bioprocess development has started in collaboration with five European biotech companies and three other academic partners (Denmark University of Technology, Technische Universität Berlin and University of Newcastle). The Division will supervise two PhD students in the project and focus is on sensor development (www.bio-rapid.eu).
The work flow in the BIORAPID project.

**Conceptual design methodology**

The division continues the successful research on conceptual design previous developed together with Prof. Mats Björkman (IEI/LITH) for which we have created the name biomechatronic design (Mandenius and Björkman, Biomechatronic design for biotechnology, Wiley and Sons, 2011). The methodology provides efficient methods and tools for the design of technical systems that merge biological, mechanical and electric components. During 2014 we have expanded the methodology to new applications and refined the methodology for bioprocessing and bioanalytics. A recent study has been published on biomechatronics applied to cardiomyocyte production (Darkins and Mandenius, 2014).

**Operator training simulators**

The PhD project on operator training simulators (OTS), previously with focus on engineering education, has taken an important step towards use in industry. With support from Lantmännen Stiftelse we apply the OTS methodology to operator training in a bioethanol plant. During 2015 a system is planned for use within a full scale manufacturing unit.

Furthermore, during 2014 an OTS application on recombinant protein production was published by our team (Gerlach et al, 2014).

**NEW COLLEAGUES**

Gunnar Hörnsten has been appointed new adjunct professor in engineering biology, especially analytical biotechnology. He is CEO of Ceffort AB and previously docent at IFM. Gunnar is responsible course leader and examiner for the CDIO master course Design of Biotechnical Process and Production Systems.

Danny van Noort has been appointed new associate professor in engineering biology. He provides valuable competence in microfluidic design to the division and support in supervising PhD students. Danny received his PhD at IFM 1999. He is also presently associate professor at Universidad de los Andes, Santiago de Chile.

A virtual bioreactor for operator training and for teaching master students in engineering and chemical biology.
Chemical and Optical Sensor Systems

STAFF

Professors: Ragnar Erlandsson and Helen Dannetun (Rector at Linköping University), Martijn Kemerink
Associate professors: Mats Eriksson, Daniel Filippini
Assistant professor: Stefan Welin Klintström (head of the division)
Researcher: Dr Anke Suska
Research engineers: Hans Sundgren and Bo Thunér (lab manager)
Administrative staff: Anna Maria Uhlin
Post-doc: Mikhail Vagin
PhD students: Roger Klingvall, Alina Sekretarova, Hassan Abdalla, Nikolaos Felekidis, Guangzheng Zuo

GENERAL INFORMATION

The research within the Division of Chemical and Optical Sensor Systems (CheOpS) is multidisciplinary. The projects are often conducted in collaboration with other divisions within the three scientific branches of Applied Physics, Material Science and Chemistry. 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 the VINNOVA-funded: Forum Securitatis, a graduate school in security research.

The research groups within the Division of Chemical and Optical Sensor Systems are led by:

• Ass prof Mats Eriksson
• Ass prof Daniel Filippini
• Prof Martijn Kemerink

Research group Martijn Kemerink – Complex Materials and Devices

Organization – This group was initiated January 2014 and will focus on the study and development of novel devices for predominantly energy harvesting, but also for e.g. data storage. As device functionality will depend on both the device architecture and the active material(s), also material science, mostly targeting electrical properties, will be part of our research activities.

Research – The first PhD student of the group, Hassan Abdallah has succeeded in finding an explanation for the often-observed but ill-understood ‘universal scaling’ of the field- and temperature-dependent conductivity of disordered (semi)conductors.

Universal scaling of PEDOT:PSS conductivity. Using numerical simulations, we have shown that this behaviour can result from charge carrier hopping in a disordered energy landscape. Measurement by K. van de Ruit, TU/e, unpublished.

The second PhD student of CoMaDe, Nikolaos Felekidis, has unravelled the composition dependence of ternary organic photovoltaic (OPV) blends and investigated the excitation energy dependence of charge separation in OPV devices.

PhD student Guangzheng Zuo and research assistant Olof Andersson started in September on, respectively, ratchet devices and thermoelectric materials.

Research group Daniel Filippini – Optical Devices Lab

Daniel Filippini’s group works on optical and 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) (P. Preechaburana, A. Suska, D. Filippini, Trends in Biotechnology 32 (2014), 351-355).

The other main research focus is microfabrication methods for disposable optics and fluidics. The simplification of microfabrication techniques used for lab-on-a-chip (LOC) development is central to accelerate optimization cycles and to disentangle design from cost constraints. Thus, device architectures could be explored and evolved with unprecedented freedom.

In 2014, Filippini’s group demonstrated the first Unibody-LOC (ULOC) fast micro-prototyping concept, which entirely transfers complex fabrication tasks to a 3D printer. ULOCs are designed around a single monolithic 3D printout (unibody), which integrates connectors, microfluidics and detection regions. (G. Comina, A. Suska, D. Filippini, Lab Chip 14 (2014), 2978-2982). ULOCs can be produced in less than 10min, at an average cost of 0.5 US$.

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” has been a project financed by Formas during 2011-2014. In this project, new sensors with improved properties for drinking water monitoring, such as improved detection limits and faster response times have been developed.

Alina Sekretaryova, PhD student, has during 2014 written and defended her Licentiate thesis “Novel reagentless electrodes for biosensing”.

The group has furthermore been involved in a project within the VINNOVA program “Challenge-driven innovation”. The project name is “Online sensor system for resource-efficient water management (Sensation)”. The role of the Eriksson group was to provide “electronic tongues and noses” for online water monitoring in field tests, in particular for detection of microbial contaminations and petroleum products. One of these sensors is the self-polishing electronic tongue illustrated in the figure below.

Molecular Physics

STAFF

Professors: Bo Liedberg (on leave)
Associate professors: Thomas Ederth (Acting head of division), Karin Enander, Daniel Aili
Assistant professors: Jaywant Phopase, Johan Hurtig (on leave)
Post-docs: Ana Villamil Giraldo, Staffan Dånmark, Sushanth Gudlur (co-financed with Sofia Ramström, IKE), Erik Martinsson, Robert Selegård
PhD students: Feng-I Tai, Abeni Wickham, Wëtra Yandi, Christopher Aronsson, Camilla Sandén, Mohammad Javad Jafari, Ranjithkumar Ravichandran, Petter Sivlér (Industry PhD student, Sz2Medical AB)
Administrative and technical staff: Therese Lindkvist, Malin Wahlberg, Anna Maria Uhlin, Bo Thunér

SUMMARY

The multidisciplinary research in the division is connected via some common themes in biologically inspired surface and colloid science: Biosensing and biochip technology, antifouling surfaces, molecular self-assembly, spectroscopy of organic thin films, and nanoscale plasmonics.

Biomolecular recognition. We develop new recognition molecules for biosensing, such as peptide-based substrate mimics for proteolytic enzymes for colorimetric sensing. We also characterize protein-protein interactions and work to design sensor surfaces in order to allow for these interactions to be correctly interpreted

Self-Assembly techniques are used to produce novel architectures and materials, on surfaces and in bulk.

Self-assembled monolayers (SAMs) are both subjects for basic studies of structure and properties, and explored as tools for design of functional surfaces. Molecular self-assembly of responsive peptide-based hybrid materials is utilized for colorimetric sensing and for fabrication of supramolecular hydrogels.

Plasmonics Activities involve fundamental studies of metal-enhanced fluorescence and properties affecting refractive index sensitivity of plasmonic nanoparticles and nanoparticle assemblies, as well as the use of localized surface plasmon resonance (LSPR) for biosensing (Fig 1) or improved imaging of adsorption phenomena via nanoparticle arrays on surfaces.

Figure 1. Peptide-coated gold nanoparticles aggregated into a cluster. Specific interaction of the peptide with particular proteins prevents aggregation, with ensuing visible differences in optical absorption, thus acting as a biosensor.
Synthesis of peptide libraries for identification of novel biorecognition elements (K. Enander, R. Selegård)

With the ambition to meet needs for small, robust recognition elements in several projects within the divisions of Molecular Physics (D. Aili) and Molecular Surface Physics and Nanoscience (K. Uvdal and C. Brommesson), we are currently setting up procedures for solid phase synthesis of large peptide libraries, based on the one-bead-one-compound approach. High-affinity recognition peptides for protein targets are selected by a colorimetric screening assay and sequenced by MALDI-TOF-MS.

Figure 3. Brightfield image (top), surface plasmon resonance image (middle) and an overlay (bottom) of diatoms (*Navicula incerta*). The SPR image shows the attachment points to the surface, and can also be used to quantify adhesive deposits or slime production.

Teaching

We teach at undergraduate and graduate levels in courses related to our research areas: Supramolecular chemistry, Molecular physics, Surfaces and interfaces, Proteomics, Materials in medicine, Fluorescence spectroscopy. Karin Enander is vice chair of the study board for chemistry, biology and biotechnology.

**HIGHLIGHTS**

**Biomaterials (Daniel Aili)**

We design and synthesize components and materials for tissue engineering and drug delivery applications. We have, among others, developed a number of polypeptides that fold into heterodimeric parallel coiled-coils with affinities for dimerization spanning over four orders of magnitude. The peptides undergo social self-sorting when mixed and are investigated as components in supramolecular hydrogels. We have also developed a method for photochemical synthesis of gold nanoparticles inside liposomes and methods to tune liposome permeability using competitive peptide-folding and membrane partitioning interactions. In collaboration with Sofia Ramström (Faculty of Health Sciences, LiU), we investigate collagen modifications on platelet activation and aggregation.

**Biosensors (Daniel Aili)**

We have continued our efforts to develop sensitive and robust nanoplasmonic biosensors (Figures 1 and 2). A generic concept for colorimetric detection of phosphatase activity, based on zinc-mediated aggregation of polypeptide-modified gold nanoparticles, was established. We have also investigated and reported on numerous methods to improve the sensitivity of refractometric sensors based on plasmonic nanoparticles. In particular, the effect of surface immobilization and presence of surfactant bilayers on sensor performance have been characterized in detail in collaboration with the groups of Chad Mirkin and George Schatz (Northwestern University, USA). A Vinnova funded collaborative project (together with KTH, Alzecure, and KI) on sensor development was also initiated, aiming at in vivo detection of disease biomarkers.

**Figure 2. Principle for affinity-based plasmonic sensing using LSPR. Adsorption of the analyte changes the local refractive index near the particle, inducing a change in the plasmonic resonance.**

**Figure 3.** Brightfield image (top), surface plasmon resonance image (middle) and an overlay (bottom) of diatoms (*Navicula incerta*). The SPR image shows the attachment points to the surface, and can also be used to quantify adhesive deposits or slime production.

**Figure 4.** Brightfield image (top), surface plasmon resonance image (middle) and an overlay (bottom) of diatoms (*Navicula incerta*). The SPR image shows the attachment points to the surface, and can also be used to quantify adhesive deposits or slime production.

**Marine biofouling (Thomas Ederth)**

Fundamental aspects of bioadhesion of marine organisms are investigated using molecularly engineered model coatings. Recent work on the antifouling properties of lactose-based SAMs extends previous work demonstrating that antifouling properties of saccharides depend on both sugar type and SAM structure in complex ways. Work dissecting the effects of polymer structure on the antifouling properties include both brush structural studies, hydrogel coatings and charge-balanced polymer gradients. We also develop optical methods for real-time investigation of the dispersive stages (spores, larvae) of marine organisms, for qualitative and quantitative studies of surface colonization. Our latest contribution is integration of imaging SPR in a fluorescence microscope (Figure 3).
Mechanisms of lysosomotropic detergents (Thomas Ederth, Ana Villamil Giraldo)

Lysosomes are vesicular organelles containing hydrolytic enzymes 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), Atul Parikh (UC Davis) and Timmy Fyrner (Northwestern University) we use biophysical tools to investigate how lysosomotropic detergents destabilize lysosomal membranes, and also how they can be used as vehicles for lysosome-specific delivery.

Interfaces in Organic Electronics (Thomas Ederth)

In collaboration with groups at LiU specialized in organic electronics (Inganäs, Berggren) we develop procedures for *in situ* infrared spectroscopic characterization of polymeric materials and devices under electrochemical control, such as monitoring of ionic charge carrier (re)distribution at electrode interfaces in electrochemical light-emitting transistors (Fig 4), and studies of the charge storage mechanisms in polypyrrole/lignin electrodes.

Regenerative Medicine

**STAFF (WITHIN IFM)**

*Professors*: May Griffith, Kajsa Uvdal, Peter Konradsson, Anthony Turner, Bo Liedberg (on leave)

*Associate professors*: Edwin Jager, Guannan Wang

*Assistant professors*: Jaywant Phopase, Martin Mak

*Postdocs*: Amy Gelmi, Sushanth Gudlur, Ayan Samanta

*Senior research associates*: Hirak K. Patra, Chyan-Jang Lee

*PhD students*: Abeni Wickham, Ranjithkumar Ravichandran, Mårten Skog, Mattias Tengdelius.

**SUMMARY**

The regenerative medicine group at IFM is part of the larger Integrative ReGENerative Medicine (IGEN) Centre, a strategic initiative at Linköping University (LiU), inaugurated in May 2010 to bridge the translational gap from bench to bedside in the area of regenerative medicine, as well as to strengthen collaborations between the technical and health science faculties at LiU.

As such, IGEN focuses on strengthening the translational research capacity within Linköping through supporting multidisciplinary studies combining biomaterials research, chemistry, nanotechnology, stem cell biology and non-invasive imaging and biosensor techniques to develop implants and follow their progress after grafting into hosts. We have focused our efforts in cornea, skin and cardiovascular regeneration.

A laboratory for production and physico-chemical characterization of biomaterials is hosted at IFM by the Division of Molecular Physics.

**HIGHLIGHTS**

**External Review** In 2014, all the strategic research centres at LiU including IGEN underwent external review. IGEN was commended in particular for its translational work in cornea regeneration.

**Research Funding** IGEN researchers from IFM and the Health sciences campus were successful in obtaining funding for translational regenerative medicine research in 2014. Funding that involves IFM researchers includes a 24 MSEK framework grant in clinical therapy research from the Vetenskapsrådet to Per Fagerholm, May Griffith and Ankica Babic. This is for multi-centre evaluation of a biosynthetic cornea optimized by IGEN researchers. May Griffith, Folke Sjöberg and Nathaniel Robinson (IFM, Transport and Separations Group) along with collaborators from Uppsala University also received funding from the Vetenskapsrådet for a project to regenerate skin after full thickness burns.

**Research Highlights** In 2014, we have had new materials developed by Asst. Prof. Jaywant Phopase and his team in pre-clinical testing in large animals at Adlego AB, a testing lab recognized by the Swedish Medical Products Agency. Figure 1 shows an implant and an implant within a cornea.

![Figure 4. We use infrared microscopy to monitor ion distributions and redox processes in electroactive polymers. The image shows the distribution of triflate ions in a light-emitting electrochemical cell, as determined from the intensity of the asymmetric sulfonate stretching vibration.](image-url)
Jaywant Phopase’s team has manufactured implants for clinical evaluation in a cleanroom under GMP for clinical trials. Martin Mak and his group have recently completed a study to reliably encapsulate single cells for delivery with controlled release, and are looking forward to testing in animal models in 2015. Anthony Turner, Martin Mak and May Griffith continue to make progress in their development of a theranostic contact lens. For their model lens, they have shown that they can detect inflammatory cytokines and release an anti-inflammatory drug. PhD student Mattias Tengdelius continues with synthesis of fucoidan mimics, and published his first paper in Biomacromolecules. As well, we have first-authored publications from PhD student Abeni Wickham on electrospun meshes incorporating carbon nanotubes as potential cardiac patches (Fig. 2), and anti-viral strategies by exogeneous application of anti-viral peptides and gene transfer by senior research associate, Chyan-Jang Lee.

More details on regenerative medicine at LiU, including upcoming courses and meetings can be found on the IGEN web-site: www.liu.se/igen.

Molecular Surface Physics and Nano Science

STAFF
Professor: Kajsa Uvdal
Junior researchers: Xuanjun Zhang, Caroline Brommesson
Postdocs: Zhangjun Hu, Guannan Wang, Qiong Zhang
PhD students: Maria Ahrén, Natalia Abrikossova, Andreas Skallberg, Emanuel Larsson and Peter Eriksson
Technical staff: Bo Thunér
Administrative staff: Therese Lindkvist

GENERAL INFORMATION

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 nanoprobes for biomedical imaging. Biospecific binding phenomena at solid surfaces are investigated. Design and characterization of new and improved nanoprobes 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 transition metal and 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) and computed tomography (CT) at the synchrotron facility at Elettra Trieste in Italy.

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) and computed tomography (CT). This project includes material design and synthesis, characterization, surface modification, biofunctionalization and signal optimization followed by tagging for targeting purposes. 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. CT is done at Elettra Italy. 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.

Figure 1. A) Transmission electron microscope images of one Eu doped Gd₂O₃ based nanoparticle on a SiOₓ surface B) Schematic illustration of one surface modified nanoparticle C) strategy for surface modification D) MR image of the human brain.

Promising data on CT is just obtained. 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. The material developed has high potential both as CT nanoprobes and as a positive MR contrast agent. We have initiated and established a spin off company Spago Imaging AB.

Nanoparticle surface modification strategies are of main importance. We have now, in collaboration with P. Norman, M Linares Theoretical Chemistry, Linköping University and obtained theoretical calculations, verifying the experimental based assignments and vibrational assignments and molecular coordination for functionalized surfaces and nanoparticles.

Core level imaging spectroscopy NanoESCA
A new combined PEEM and imaging XPS equipment (NanoESCA) financed by KAW is recently installed in our laboratory. The NanoESCA instrument deliver images chemical information with lateral resolution on the micro- and nanolevel. A set of images from Core level imaging spectroscopy NanoESCA on Bifunctional gadolinium decorated ZnO nanocrystals, stamped on SiOₓ surface, are shown in Figure 3 a–c.

Figure 2. NanoEsca images of Bifunctional gadolinium decorated ZnO nanocrystals transferred to a silicon surface using a polydimethylsiloxane (PDMS) stamp to produce micro-patterns with a diameter of 80 μm. a) Photoemission electron microscopy (PEEM) image b) XPS in imaging mode for core levels C1s, Si2p and Gd3d₅/₂ c) XPS in imaging mode of two chemically different O1s.

Momentum microscope with a HeI lamp (21.2 eV) was installed, as an additional tool for surface analysis. This microscope is desired for imaging the angular distribution of emitted electrons, i.e. k-space imaging. Real space and k-space imaging of Ag(111) is shown in Figure 1 resp. Figure 2. For k-space, the image is taken at photon energy of 21.2eV, showing emission of valence electrons close to the fermi energy. The white spot in the center of Figure 2 represents the surface state.

Figure 3. Real space imaging of Ag(111), FoV 81μm with an desired area determined by the iris aperture Figure 2. K-space imaging of Ag(111) with a FoV 5.2 Å⁻¹.

Figure 2. NanoEsca images of Bifunctional gadolinium decorated ZnO nanocrystals transferred to a silicon surface using a polydimethylsiloxane (PDMS) stamp to produce micro-patterns with a diameter of 80 μm. a) Photoemission electron microscopy (PEEM) image b) XPS in imaging mode for core levels C1s, Si2p and Gd3d₅/₂ c) XPS in imaging mode of two chemically different O1s.
**Highly sensitive and selective molecular probes for metal ions sensing**

Novel fluorescent molecular probes were strategized and synthesized for the detection and visualization of trace metal ions. They are derived from rhodamine B, which is an ideal substrate for the construction of “on” or “off-on” molecular probes for analyzing the analytes in the environmental or biological systems, due to long emission wavelength (> 550 nm) of its ring-opening form. Among them, the selective FRET-based ( Förster resonance energy transfer) ratiometric “off-on” fluorescent probe for Cu²⁺ was strategized and synthesized by using a facile “click” reaction. The ratio of dual emission intensities exhibits a drastic 28-fold enhancement upon addition of Cu²⁺. In this work, the probe has been successfully tested in cellular studies for ratiometric fluorescent visualization of intracellular Cu²⁺ with almost no cytotoxicity. These works will be of guiding significance to our strategizing the multi-modal probes for tracking analytes in the biological systems.

**RESEARCH COLLABORATIONS**

Prof A Persson Center for Medical Image Science and Visualization (CMIV). Prof O Gimm, Health University Linköping, Prof P. Norman, Theoretical Chemistry, LiU Prof, R. Yakimova, Material Physics, Prof. A. Lloyd Spetz, Åbo Finland, T Bengtsson Örebro, LiU Cancer network, IGEN centre which is strategy area of regenerative medicine University SPAGO Imaging AB Lund. MaxLab Swedish National Laboratory in Lund, S. S. Venkatraman NTU Singapore J Tromba Elettra Trieste Italy. C Dullin Germany

**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 undergraduate education in this scientific area. K. Uvdal is the director of CeNano.

www.ifm.liu.se/applphys/surfnano/
Surface Physics and Chemistry

**STAFF**

**Professors:** Mats Fahlman (Head of Division)

**Associate professors:** Nathaniel Robinson (Assistant Head of Division), Koung-An Chao (Emeritus), William R. Salaneck (Emeritus)

**Research engineers:** Slawomir Braun, Xianjie Liu

**Post docs:** Abdelmalek Ainsebaa, Shengwei Shi, Zhengyi Sun

**PhD students:** Qinye Bao, Katarina Bengtsson, Per Erlandsson, Sara Nilsson, Chuanfei Wang

**Administrative staff:** Kerstin Vestin

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**SUMMARY**

The division consists of two research groups: Organic Physics (Fahlman, Bao, Braun, Liu, Shi, Sun, Wang) and Transport and Separations (Robinson, Ainsebaa, Bengtsson, Erlandsson, Nilsson).

The Organic Physics research consists of fundamental study and model development of weakly-interacting organic-organic and organic-metal interfaces; interface engineering in organic electronics i.e. development of techniques for improving charge injection, exciton dissociation 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: the effect of synthesis and choice of (poly)anion on conductivity, bio-compatibility and general surface properties. The Organic Physics group also does research focused on the study and design of hybrid organic spintronic interfaces (spinterfaces) with the aim to understand and improve spin injection/detection.

The Transport and Separations group focuses on ionic and electronic transport in fluids and solid-state materials. One particular goal of the research is to create and understand new devices in areas such as micro- and nano-fluidics and solid-state lighting. The group develops systems for chemical, biological and medical study using microfluidic labs-on-chips. In addition to the work on microfluidics, research and development of light-emitting electrochemical cells are carried out in collaboration with Umeå University.

External collaborations with specific funding during 2014 included the EU-FP7 project Next Generation Hybrid Interfaces for Spintronic Applications (HINTS), the EU-FP7 project SUstainable Novel FLexible Organic Watts Efficiently Reliable (SUNFLOWER), the SSF project Large-area light-emission on the roll.

The division received additional funding from three contracts issued by the Swedish Research Council (VR), a contract (Designed Nanoparticles by Pulsed Plasma) from the Knut and Alice Wallenberg foundation and the Göran Gustafsson Foundation for Research in Natural Sciences and Medicine. Further funding was received internally from the LiLi-NFM Linnaeus project and the AFM project.

The division’s involvement in the undergraduate teaching activities of the university during 2014 consisted of the course THYA46 Engineering Project (Bengtsson).

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**HIGHLIGHTS**

**Organic Physics Group**

We have developed a general model treating the effects of doping and intermolecular order on energy level alignment at organic and hybrid organic heterojunctions. (OrgEl)

We have studied the effect of integer charge transfer states at organic donor-acceptor interfaces allowing us to formulate new design rules for minimizing open circuit loss in organic bulk heterojunction solar cells. (Åbo Akademi)

By combining XPS, UPS and NEXAFS, we studied the chemical interactions, energy level alignment and degradation effects of materials and interfaces in ternary and tandem organic bulk heterojunction solar cells (GenesInk, University Jaume I, Chalmers, CNRS, AGFA-Gaevert in SUNFLOWER).

Aided in the development of various carbon and transition metal nanostructures using surface science characterization techniques (IMEC, University of Hasselt, CNRS, Max Planck)

By combining XPS, UPS, NEXAFS and XMCD, spininjected hybrid organic interfaces were designed and studied (HINTS and Fudan collaboration).

**Transport and Separations Group**

Continued its progress in developing “soft” (e.g. polymer) systems for electronic, chemical, and biological applications, including projects developing sacrificial template materials for 3D printing microfluidic devices, and cell delivery systems for microfluidic bioreactors, creating scalable gel electrophoresis systems by using pi-conjugated polymers for electrodes, and creating hybrid nanoparticle/polymer devices for efficient flexible lighting.
Increasingly used 3D printing in our own research, and now support other groups interested in testing the technology for use with soft and/or conducting materials.

NDR led Work Group 1 in the COST targeted network Sci-Generation (www.scigeneration.eu) working to enhance the European research environment for the next generation of young scientists.

COOPERATING PARTNERS AND VISITING SCIENTIST

The different international universities, institutes and companies with which funding were shared in projects during 2014 are listed below:

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, Merck, DuPont Teijin Films, AMCOR Flexibles, AGFA-Gaevert NV, Fluxim AG, Belectric OPV, SAES Getters, CNR – ISMN, Fachhochschule Nordwest Schweiz, Chalmers, FhG IVV & ISC, Universitat Jaume I de Castellon, GenesInk, CNRS, University of Antwerpen.

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 and its subsidiaries, LunaLEC AB and LunaMicro AB.

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

STAFF

Head of division: Agneta Johansson

Professors: Mats Amundin (Adjunct professor), Per Jensen, Jan Landin (Emeritus), Matthias Laska, Per Milberg

Associate professors/Senior lecturers: Agneta Johansson (Director of studies), Jordi Altimiras, Johan Edqvist, Karl-Olof Bergman, Jenny Hagenblad, Anders Hargeby, Matti Leino, Ronny Lock, Karin Tonderski, Jennie Westander (adjunct), Dominic Wright, Thomas Östholm

Assistant professors: Hanne Løvlie, Lina Roth, Lars Westerberg

Junior lecturers: Kjell Carlsson, Eva Mattson, Åsa Rybo Landelius

Guest researcher: Els Willems, Natasa Costermans, Anouschka Middelkoop

Post doc: Carlos Guerrero Bosagna, Rie Henriksen, Niklas Jansson, Dennis Jonason

PhD-students: Beatrix Agnvall, Johan Beltéky, Magnus Elfving, Maria Ericsson, Amir Fallahshahroudi, Nils Forsberg (NTU), Perrnilla Foyer (FHS), Andrey Höglund, Karin Johannesson, Martin Johnsson, Anna-Carin Karlsson, Caroline Lindholm, Maria Lundström, Pia Lötvedt, Helena Olsson, Mia Persson, Ann-Sofie Sundman, Josefine Zidar, Hanna Österman

Administrative/Technical staff: Petros Batakis (Lab Technician), Ann-Charlotte Svensson-Holm (Lab Technician), Lejla Bektic (Animal Technician), Tove Bjerg (Technician), Eva-Maria Stigsdotter (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, who is also the director of studies, and three assistant heads of division. This group meets weekly and is responsible for matters concerning budget, teaching, research, PhD-education and organization.

Within IFM Biology, 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 2014 present their activities.

The PhD-education is carried out within four different subjects: Ecology, Zoology, Ethology and Genetics. Within Ecology, emphasis is on community and population ecology, including conservation biology, vegetation and wetland ecology. In Genetics, research training is focusing on the domestication of plant and and animal species. In Zoology, research is mainly focused on developmental aspects of cardiovascular control and comparative olfaction research, and in Ethology, focus is on domestication effects on behaviour in chickens and behaviour genetics and welfare in chickens and dogs. The staff is also deeply involved in undergraduate teaching in all subjects covering the biological education programs.

IFM Biology has had a great success rate in external funding over the last couple of years, and important grants were also obtained 2014. For example, researchers from the branch were awarded project grants from VR. Professor Per Jensen, professor Per Milberg, and Senior lecturer Jordi Altimiras hold contract supports from the University. Furthermore, Professor Per Jensen is supported by an ERC Advanced Researcher Grant.

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

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 AVIAN group. Their behaviour, genomics and physiology are studied in a number of research projects.
The A VIAN Group performs research including amongst other topics in biology, ethology, personality, epigenetics, genetics, physiology, evolution and welfare issues. The P.I.s in the group currently includes Per Jensen (head), Jordi Altimiras, Dominic Wright, Hanne Lovlie, and Urban Friberg.

Traditionally has research of the group mainly focused on the ancestral Red Junglefowl and modern chicken breeds with the goals of understanding the genetic basis of animal domestication and its functional mechanisms. More recently has the research expanded to include also other avian species (Tinamou), mammals (dog), and insects (Drosophila).

As part of the Centre of Excellence in Animal Welfare Science our research is also dedicated to the improvement of animal welfare. During 2014, we published the most extensive mapping of hormonal and behavioural responses to stress in chickens, showing that domestication has significantly modified several aspects of the stress reaction (Ericsson et al 2014, Phys Behav).

The ethology lab under Per Jensen has continued work showing that Red Junglefowl selected for low fear of humans displays correlated responses in a number of other behaviour traits. A study was published showing that such selection improves dominance and reproduction in the low-fear birds (Agnvall et al 2014, Animal), and another where it was demonstrated that the large sex differences in behaviour of chickens can to a large extent be attributed to epigenetic effects (Nätt et al 2014, PLoS ONE). The epigenetics work of the group is being developed largely by Carlos Guerrero-Bosagna. Within the framework of an Advanced Grant from ERC (“GENEWELL”), Jensen’s group studies the effects of epigenetics on stress in both chickens and dogs. During the year, significant advances have been made in both areas, and important publications on both species are under way. In the dog part of the project, life-long consequences of early experiences have been reported (Foyer et al 2014, App Anim Behav Sci), and further emphasis has been placed on the genetic basis for variation in dog-human contact behaviour.

Hanne Lovlie and her group continued their work exploring the causes and consequences of variation in animal personality. Articles published includes the influence of personality on establishment of social status (Favati et al 2014, PloS ONE), how an individual’s social roll can affect personality (Favati et al 2014, Proc Roy Soc B), mitonuclear genetic effects on personality (Lovlie et al 2014, Proc Roy Soc B) and female indirect mate choice strategies (Lovlie et al 2014, Anim Behav).

The genetics lab under Dominic Wright expanded with a new PhD student, and Dominic was promoted to Associate Professor and awarded a 5 year LiU Career contract. The group continue to work on the genetic basis of a sexual ornament, the comb, as well as identifying genes affecting a range of phenotypes, from behaviour to feather colour. Analysis on samples collected from Hawaii has now been performed with mitochondrial and phenotypic data indicating that the chicken population on the island of Kauai is an admixed population consisting of birds of both Red Junglefowl and domestic origin. Furthermore, selective sweeps relating to the process of feralisation (domestication in reverse) have been identified.

Jordi Altimiras and the physiology lab are currently focusing on the welfare consequences of severe feed-restriction in broiler breeder commercial chickens. This is in collaboration with the largest Swedish company in the sector SweHatch AB, financially supported by FORMAS. On farm studies of behaviour and physiology of broiler breeders before reaching sexual maturity are revealing interesting phenotypic differences associated to differential growth. Work on the mechanisms and consequences of heart size in birds continued, and new collaborations set up (the groups of Roberto Nespolo at Universidad Austral de Chile in Valdivia, and Pablo Sabat’s at Universidad de Chile in Santiago). Our first published paper using cultured chicken cardiomyocytes appeared this year in Physiological Reports. We showed that thyroid hormone is not involved in cell differentiation unlike what is known from mammalian cells. In PLoS ONE we have given evidence that the expression of the alpha-adrenergic receptor ADRA2C, putatively involved in domestication by previous studies, is not different in different brain regions and the adrenal glands of egg-laying chickens than the wildtype Red Junglefowl.

LU Research Fellow Urban Friberg joined the A VIAN group this year. His group uses the model organism Drosophila melanogaster to study the genetic basis of sexual dimorphism and the evolution of ageing. During the year a new Drosophila lab was built and several experiments were initiated.

Further information, news and publications from the A VIAN group can be found at http://www.ifm.liu.se/biology/zoology/avian/
The Sensory and Behavioral Physiology Group

**Professor:** 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 neuroanatomical and genetic properties such as the size of olfactory brain structures or the size of the olfactory receptor repertoire. A third research topic includes studies on the effects of behaviorally relevant odors on the behavior of animals. Here, particular emphasis is on food odors, social odors, and predator/prey odors. With all three topics, a comparative approach including human subjects and a variety of animal models is employed.

In collaboration with the Universidad Veracruzana in Mexico, Jenny Larsson and Anna Maitz showed that spider monkeys perceive the taste of proteinogenic amino acids in a similar manner as human subjects do. More specifically, the spider monkeys preferred certain amino acids described as “sweet” by humans over tap water, and they generally rejected certain amino acids described as “bitter” by humans. Further, the spider monkeys were able to detect some of the amino acids at concentrations in the millimolar range, suggesting that the taste of these substances may affect their food choice. (Larsson, Maitz, Hernandez Salazar, and Laska 2014. Physiol Behav 127: 20-26.)

A spider monkey (Ateles geoffroyi) drinking from one of two simultaneously presented bottles in a taste test. The study took place at the field station of the Universidad Veracruzana in Mexico.

**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. 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. The group is also collaborating with the research division of AFB International, one of the largest pet food companies in the United States, performing joint studies on taste perception in pet animals. Finally, the group is collaborating intensively with Kolmården Wild Animal Park where numerous studies are performed.

**HIGHLIGHTS**

Matthias Laska and two of his students were able to demonstrate that a single compound found in the odor of mammalian blood can be as efficient in eliciting behavioral responses in large carnivores as the odor of real blood. More specifically, they showed that Asian wild dogs, African wild dogs, South American bush dogs, and Siberian tigers displayed the same high degree of interest towards wooden logs impregnated with the blood odor component trans-4,5-epoxy-(E)-2-decenal as towards wooden logs impregnated with real horse blood. In contrast, wooden logs impregnated with a fruit odor component or with a solvent were significantly less interesting to all four carnivore species. This suggests that trans-4,5-epoxy-(E)-2-decenal may be perceived by predators as a “character impact compound” of mammalian blood odor. (Nilsson, Sjöberg, Amundin, Hartmann, Buettner, and Laska 2014. PLoS ONE 9: e112694.)
Research during 2014 focused on species-rich grasslands and deciduous forests and involved plants and insect. We published a study showing how efficient pheromone traps can be within conservation, both by finding important by difficult-to-sample parts of biodiversity and by allowing such species to be used as indicators or valuable environments. This is a step forward that both by saving resources available for conservation and for providing a fuller picture of biodiversity (most of which is difficult to sample). Our study system was the click beetle Elater ferrugineus that is dependent on hollow oak trees. Several projects with similar focus, but different approaches for sampling and analyses, are currently running.

In 2014, we attempted an additional pheromone system: a group of moths in grassland (burnet moths), that are potential indicator species for monitoring biodiversity. In two papers in 2014 we evaluated data from experiments comparing different management options for valuable grasslands, and we did so by turning biodiversity data into odds ratios, that could then be used in metaanalyses. We were able to show that the actual method of cutting grass had no effect, but that spring-burning was not a method that could be used regularly if maintaining biodiversity is the aim. Within the same theme, we started up a new project in 2014, sponsored by the Swedish Board of Agriculture.

Another paper in 2014 compared the host-specificity among saproxylic beetles, i.e. to what extent beetles living in decomposing wood prefer particular tree species. To our surprise, much species showed very little preferences.

A project that has been very exciting is our study of biodiversity of clearcut in production forests and the effect of previous land-use. It has turned out that landuse in the late 1800s had a very strong effect on today’s biodiversity. Clearcuts with a land use history of meadows had 36% more species even after at least 80 yrs of production forests than clearcuts with a history as forests.

During 2014, we continued our work involved species dependent on, or promoted by, forest fire.
Plant Evolution and Domestication Group

STAFF

Associate professors: Johan Edqvist, Jenny Hagenblad, Matti Leino
Post doc: Per Larsson
PhD students: Nils Forsberg, Maria Lundström
Technicians: Tove Bjerg, Ida Gustafsson
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 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, headed by Jenny Hagenblad and Matti Leino explores the genetics and evolution of landrace crops and agricultural history with particular attention to crops cultivated in Fennoscandia. Genebank material, seed samples from historical collections and archaeological remains are used for the studies and both population genetic structure and specific traits such as flowering time and nutrient content of historical crops are explored.

HIGHLIGHTS

The LTP group has published the first characterization of LTPs from non-flowering plants. We also published evidence for that LTPs are required for the development of seed coats and pollen in Arabidopsis.

Per Larsson has joined the Historic Seed Group group as a postdoc and Maria Lundström as a PhD student. The group has published several papers in both English and Swedish speaking journals. The paper describing historical barley farming in Fennoscandia was featured in the Heredity podcast for September. Maria Lundström has visited Robin Allaby’s lab in Warwick for work with archaeological crop material. Matti and Jenny have visited Gran Canaria and Tenerife and presented results from collaborative research projects there.

COLLABORATIONS

External Collaborations

LTP group: Tiina Salminen (Åbo Akademi University), Peter Mattjus (Åbo Akademi University), Magnus Eklund (Uppsala University)

Historic seed group: Robin Allaby (University of Warwick), Robbie Waugh and Joanne Russell (James Hutton Institute, Scotland), Anna Palmé (NordGen, Alnarp), Else-Marie Strese (Nordiska museet, Julita), Amelia del Carmen Rodrigues-Rodrigues and Jacob Morales-Mateos (Universidad de Las Palmas de Gran Canaria, Spain), Diane Lister (Cambridge University, UK), Mia Avci-Lemiainen (Turku University, Finland), Tytti Vanhala (Vanhalytix, Sweden), Agneta Börjeson (Röttle Natur & Kultur) Hugo Oliveira (CIBIO, Portugal), Jens Heimdahl (National Heritage Board) and Bente Graae (Norwegian University of Science and Technology, Trondheim)

EXTERNAL ACTIVITIES

Matti Leino and Jenny Hagenblad presented their research results at the NTAG meeting in Stockholm and Matti also gave an oral presentation at the ISBA meeting in Basel. The senior members of the group have also been evaluating three PhD dissertations.
Wetland Dynamics Group

**Docent:** Anders Hargeby

The group works on different aspects of wetland ecology and nutrient flows. In 2014, we have carried out a pilot mesocosm study on the effects of liming on plankton and dissolved phosphorus in the eutrophic lake Tåkern. This showed that the phytoplankton biomass was reduced, but not for more than two weeks. There was no detectable effect on the dissolved phosphorus, which remained at low (<5 ug L⁻¹) concentrations in all treatments.

Mesocosms in Lake Tåkern, used to study the impact of liming on phosphorus concentrations and the plankton community. Photo: Claire Froger

Anders Hargeby has also developed a protocol for laboratory rearing of aquatic isopods, mainly *Asellus aquaticus*, which is used as a model organism to study evolutionary processes in shallow waters.

A different research direction focuses on particle and phosphorus retention in wetlands and streams. Here, two studies have been started up in 2014. One focuses on the effect of settling ponds upstream filters for sorption of phosphorus in agricultural runoff, and is part of a remediation project on Ingarö initiated by the Foundation BalticSea2020. The aim of the other is to evaluate the retention in two stage ditches as a function of established plant community at different locations along the ditch.

Creation of two stage ditches is an attempt to recreate the natural profile of streambeds with the ecosystem services that may be provided, such as P retention on the terraces created. Photo: K. Johannesson

Finally, we have evaluated the use of a chemical pre-treatment method for separating out nitrogen and phosphorus in biofertilizers from biogas plants. This is part of a Biogas Research Centre (BRC) systems analysis of different approaches to a more efficient recycling of such nutrients to arable land or possibly future production wetlands. The project involved cooperation with BRC partner companies and with IEI, Environmental technology and management at LiU.

**COOPERATION**

Our projects involve cooperation with the University of Lund, Sweden; SLU (Uppsala), Sweden; Halmstad University, Sweden; SMHI, Sweden, the University of Greifswald, Germany, and LRF Östergötland, Sweden, for the two stage ditch study, as well as partners and members in Biogas Research Center.

**EXTERNAL ACTIVITIES**

Members from our group have: i) participated (as expert) in a 2-day course on “Aquatic plants” for Swedish officials responsible for monitoring of inland waters; ii) evaluated the effect of wetlands as traps for nutrients in a project led by Halmstad University for the Swedish Board of Agriculture; iii) served as Technical advisor in Sida’s program BioInnovate, supporting Biotechnology innovations in East Africa; and iv) evaluated research project applications for VR U-forsk and SLF.
General Information

STEERING COMMITTEE

Professors: Bengt-Harald “Nalle” Jonsson (Chair), Per Hammarström, Peter Konradsson

Research Divisions of Chemistry

• Protein Chemistry
• Molecular Biotechnology
• Organic Chemistry
• Physical Chemistry Inorganic
• Chemistry
• Analytical Chemistry

SUMMARY OF ACTIVITIES

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. 22 PhD students have been enrolled and 4 PhD Thesis were defended at the department during 2014. The research in the different research divisions are presented in the following sections.

Protein Chemistry

STAFF

Professors: Per Hammarström
Professors em: Uno Carlsson
Associate professors: Lars-Göran Mårtensson, Magdalena Svensson
Visiting professor: Mikael Lindgren (NTNU, Trondheim, Norway)
Senior staff scientist: Sofie Nyström
Post docs: Ina Caesar
Technician: Maria Thörnqvist
PhD students: Maria Jonson, Raul Campos Melo, Daniel Sjölander, Anna Zimdal, Alexander Sandberg
Administrator: Susanne Andersson

Molecular Chaperones

Folding in vivo is for many proteins assisted by several protein factors such as molecular chaperones. Although proteins can fold spontaneously the chaperones suppress aggregation during folding and increase the yield. In our research we aim to gain insights into the mechanism of chaperone function that is essential for the understanding of the folding mechanism and prevention of misfolding.

Fig I. Mechanistic studies of molecular chaperones including GroEL and GroES are studied in the Protein Chemistry research groups of Carlsson and Hammarström.

Protein Misfolding Diseases represent a large collection of diseases. This group includes for example the prion diseases Creutzfeldt-Jakob disease and mad cow disease; the amyloid diseases such as Alzheimer’s disease and familial amyloidotic polyneuropathy (Skellettasjuukan). All these diseases are connected to a specific protein that misfolds into alternate conformations and often forms aggregates with different structures. We are working with proteins involved in all of the mentioned folding diseases. Our objectives are also to
inhibit the formation of the toxic species of amyloid and prion diseases by using different strategies including small-molecule binding and interactions with molecular chaperones.

Figure II. Electron micrograph of amyloid fibrils of the peptide Aβ1-42 causing Alzheimer’s disease. The Aβ1-42 peptide and its various amyloid conformations are subjects for intense research in the Hammarström lab.

Thiopurine methyltransferase (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.

Lars-Göran Mårtensson in collaboration with the Department of Clinical Pharmacology at University Hospital in Linköping are studying mutants of TPMT which 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.

The research activities in molecular biotechnology have one focus 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. Another major undertaking concerns industrial biotechnology. The focus is to use modern proteomic tools in combination with protein engineering to develop efficient enzymes for use in industrial processes.

The Molecular Basis for the role of SOD in Amyotrophic Lateral Sclerosis

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 different NMR-methods in combination with hydrogen/deuterium-exchange experiments to unravel the effects of the mutations on the local dynamics in 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 at our disposal engineered protein variants with these properties separated. Our aim is thus 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.
Enzymatic Upgrading of Energy Gases 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 the enzyme human carbonic anhydrase II is to facilitate the removal of carbon dioxide from the blood it has been suggested that this enzyme can be used as biological catalysts in bioreactors designed for capturing and separating CO₂. However, there are no naturally occurring carbonic anhydrases that have high enough stability to be used in such a bioreactor. We have now produced engineered human carbonic anhydrases with vastly increased physical stability. However, these engineered enzymes will now be used to design industrial processes to upgrade energy gases (biogas from anaerobic digestion and thermal gasification) rather than processes for CCS.

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 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. Results from these studies show a clear link between neurodegenerative properties of the Aβ peptide in the central nervous system of Drosophila, and the propensity of the peptide to form prefibrillar assemblies that are characterized by exposed hydrophobic surfaces which can be probed by fluorescence spectroscopy.

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 and Cellulolytic Enzymes 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 novel enzymes that are active and stable at the various 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. In 2014 we realized such methods based on “induced differential meta-proteomics” which now allow us to identify novel enzymes with pre-determined activity for pre-determined conditions “at will”!

Enzymatic Enhancement of Sludge Digestability 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 digestability 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 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. To date we have concluded that the activity and life-time of commercially available enzymes is very limited in the biogas process. Thus, for the remains of this project we are aiming at finding out what processes are the cause for the decreased life time of the enzymes, e.g. chemical modification or proteolysis. If this knowledge could be obtained it might be possible to modify the enzymes for increased activity and lifetime by knowledge based protein engineering.

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 characterizing 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 proteinMexR 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.

Structural biology in cancer development and protection The oldest characterized oncogene, c-Myc, houses a series of fatal hotspot mutation sites leading to increased tumor development. We have characterized the structural properties of the transactivation domain which, surprisingly, adopts a molten 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 transactivating 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.

Protein Function and Dynamics  The research interests in the Lundström group are protein function, studied primarily using nuclear magnetic resonance (NMR) spectroscopy, and development of NMR methodology. Proteins that we are interested in include various kinases involved in cancer and malaria, thiopurine methyl transferase (TPMT) that metabolizes drugs used to treat leukemia and calmodulin that is important for calcium signaling. Long term goals with biological relevance are to develop kinase inhibitors in order to treat cancer and malaria and to explain the different activities of TPMT variants.

Organic Chemistry

Staff
Professors: Peter Konradsson
Associate professor: Peter Nilsson
Senior researchers: Åsa Rosenquist, Marcus Bäck, Hamid Shirani, Wu Xiongyu
Post-doc: Christine Dyrager, Therése Klingstedt, Elisabet Öberg
PhD students: Katriann Arja, Mathias Elgland, Leif Johansson, Linda Lantz, Karin Magnusson, Mattias Tengdelius, Jun Zhang, Rozalyn Simon
Administrator: Susanne Andersson

Activities
Synthesis of Functionalized Oligothiophene Derivatives with Specific Optical and Electronic Properties

By combining the features of polymers and the electrooptical 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.)

As a first instance we are synthesizing oligothiophenes that can be utilized as tools for studying biological and pathological process. The aim of these projects are mainly to provide molecular tools that can be used for real time in vivo 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 template molecules, such as amyloid fibrils, to generate materials that can be implemented with in research areas such as nanobioelectronics. Though a multidisciplinary collaboration with other researchers at IFM and ITN, we are aiming at develop novel materials that can be used for electronic release of pharmacistals, and devices that can stimulate and record cellular activity in complex environments.

![General chemical structure of functionalized oligothiophene derivatives.](image-url)
**Fucoidan-Mimetic Glycopolymers for Biomaterial Applications**

The biological properties of fucoidan are among the most diverse of all natural polysaccharides, including e.g. anti-inflammatory, antiviral, anticoagulant, antitumor, antithrombotic, and platelet activating properties. In spite of fucoids desirable properties they have been scarcely used for functionalization of biomaterials mainly due to their chemical heterogeneity, costly extractions and structural differences between different marine species and season of harvest. Tengdelius and Konradsson have developed a method for the synthesis of sulfated and non-sulfated fucoidan-mimetic glycopolymers through cyanoxyl-mediated free-radical polymerization (Figure IVA). This method is suitable for chain-end functionalization, enabling covalent linkage to form functionalized biomaterials. Assays for Herpes Simplex Virus-1 (HSV-1) infection (Figure IVB) and platelet aggregation (Figure IVC) showed that sulfated glycopolymers assert the same biological properties as commercially available fucoidan from Fucus Vesiculosus. Non-sulfated glycopolymers did not show these properties. We believe these results to be a first step towards a wider use of the biological properties of fucoidan in biomaterials.

![Figure IV](image)

**Figure IV.** A: Synthesis of fucoidan-mimetic glycopolymers. B: Inhibition of HSV-1 infection. C: Platelet aggregation assay.

**Synthesis of an azide-functionalized β-mannosyl triflate:**

An FDG precursor for PET imaging. Molecular probes for selective imaging of protein aggregates are important to advance our understanding of the molecular mechanisms underlying protein misfolding diseases. We have previously reported how the fluorescent properties of specific thiophene based oligomeric structures (Luminescent Conjugated Oligothiophenes, LCOs) can be used for the detection of Alzheimer’s disease. In this work, the synthesis of an azide-functionalized β-mannosyl triflate (azidoethyl 2-O-trifluoromethanesulfonyl-β-D-mannopyranoside) is described. The aim is to use the β-mannosyl triflate as a “clickable” precursor to 2-fluoro[18]-2-deoxy-glucose (FDG), one of the most frequently used radiotracers for in vivo PET imaging.

Concerning the synthesis, it has been shown that having a β-configuration of the glycosidic bond is necessary in order to obtain a sufficient radiochemical yield during the 18F labeling-step. Since β-mannosides are known to be difficult to obtain by direct glycosylation, a synthetic strategy was devised where the β-glycosidic bond was formed through a 1,2-orthoester rearrangement of a gluco-derivative that subsequently was epimerized to its corresponding manno-derivative. The synthesized FDG-precursor will be conjugated to alkyme functionalized LCOs, thus rendering amyloid specific PET tracers. However, the FDG-precursor is not restricted to amyloid specific ligands, but may in principle be conjugated to any suitable ligand having affinity for other biological targets.

![Figure V](image)

**Figure V**

**Synthesis of glycosylated porphyrin-oligothiophene conjugates**

Porphyrins and porphyrin-based compounds are of great interest in a vast variety of scientific areas due to their unique photophysical and biochemical properties. We have recently reported a porphyrin-oligothiophene conjugate that selectively binds to amyloid fibrils associated with Alzheimer’s disease which shows enhanced fluorescent properties as compared to previously used probes. In order to use these conjugates in intracellular applications, e.g., real time imaging and photodynamic therapy, the cellular uptake of the conjugate needs to be adequate. Glycosylation of the porphyrin-scaffold could offer the mean to meet this requirement. For this reason, a number of azidoethyl glycosides have been prepared (Glc, GlcNAc and Gal) that are readily attached to propargyl sulfonamides-linkers, on the porphyrin-scaffold, using Huisgen’s copper-catalyzed alkyne-azide [3+2] cycloaddition, i.e., the so called “click-reaction” (figure VI).

![Figure VI](image)

**Figure VI**

**Synthesis of Potassium Ion Channel openers**

Potassium ion channels are a structurally diverse family of transmembrane proteins that are modulated by voltage, cell metabolism, and calcium or receptor-mediated processes. They are important in the regulation of membrane potential, and the release of neurotransmitters, and contractility. Openers of these channels are potentially useful agents in the therapy of various diseases, such as acute stroke, epilepsy, psychoses, erectile dysfunction etc. Currently research has been focused on the voltage gated ion channel openers.
Three cores have been chosen as leads from the natural products, which are abietic acid (see figure), podocarpic acid and dehydroabietic acid. Some of them were known to be active in BK potassium ion channel. This project has been initiated and partly sponsored by LiU-Neuro and Professor Fredrik Elinder at IKE, LiU. More than 110 derivatives have been synthesized and attractive results have been achieved, and new cores have also been found which are more potent to the Kv channels after screening of thousands of compounds.

**Synthesis of Designer Drugs and Their Metabolites**

Designer drug is a hot research area and each year there are tens of new designer drugs being laid out to the market legally or illegally. It brings a great challenge to many forensic science researchers because there aren’t commercial available reference samples for the new drugs or their metabolites in the market. We have started the collaboration with Analytical chemistry (LiU) and Rättsmedicinalverket for the synthesis of MMB-CHMINACA, THJ2201, JWH018, AKB48 (Apinaca) and their metabolites (see figure). More than 25 metabolites have been synthesized, some of them have been analyzed and found to be identical to the metabolites in the urine samples and the extract of the culture medium of the human liver microsomes and designer drug.

**Development and application of electronically integrated bioionic gels 2014/2015.**

Our recent development of PEDOT derivatives has now been applied to different types of electrochemical hydrogels, based on composite blends of different conjugated polymers (CPs). They can be chemically modified to control desired properties such, pH, porosity, conductivity and charge. Successful routes for preparing nanoscale objects, using self-assembly and templated growth techniques has been described in some recent publications; Langmuir, 2014, 30(21), 6257. Synthetic Metals, 2014, 194, 170. Electroanalysis, 2014, 26(4), 739. Advanced Energy Materials, 2014, 4(1), 1300443.

Last year activities were also dedicated to the development of bioionic gels based on poly(ionic liquid)s constituted of choline derivatives. Initially the polymers showed high potential as support materials to integrate biomolecules, mainly neurotransmitters, for chemical delivery and sensing applications. One drawback of the derived polymers was that the porous size within the polymers, that is the “highway” for molecules to be transported through the polymer network could not be controlled synthetically from the initial synthetic strategies. In order to obtain materials with this critical parameter as a variable under synthetic control we choose a different building block for functionalization with choline and other ionic charged derivatives.

The main class of materials that we have found can serve for these demanding requirements are hyperbranched polyethers (HPEs). These macromolecules can be obtained with highly branched three-dimensional nanopolymeric architectures, adequate spatial cavities, numerous terminal functional groups, and convenient synthetic procedures distinguish them from the available polymers (the linear and crosslinked polymers). Further, we have found that HPEs possess excellent biocompatibility, controlled responsive nature, and ability to incorporate a multiple array of guest molecules through covalent or noncovalent approaches.

We have pursued synthesis and characterization of functionalized HPEs. A series of these polymers, with different degrees of functional groups and charge have and are investigated as ion selective membranes for electrophoretic transport and sensing applications. To optimize membrane properties such as ion conductivity, surface immobilization and water uptake, we control the intermolecular environments by manipulating the balance between hydrophobic and hydrophilic domains in HPEs. This have included interpenetrating networks of HPEs and other poly(ionic liquids), mixing HPEs with non-polar media, surfactant organized media, and to confine the HPEs to organized nanostructures with ABA-polymerization techniques.

The novel materials have shown great potential to integrate biomolecules in the latest generation of organic bioelectronic devices for chemical delivery/sensing and ion-based logic at the laboratory of organic electronics (LOE) ITN Norrköping, with two submitted papers and two patents in process.

In addition to this years activities we have also acted as consultants for the new polymer-chemistry lab at ITN Norrköping in the framework of Magnus Berggren granted KAW strategy.
Physical Chemistry

STAFF
Professor: Lars Ojamäe
Senior researcher: Edvin Erdtman
PhD students: Yuan Liu, Emil Kalered

ACTIVITIES

The research projects concern computational-chemistry studies of nanostructures, functionalized nanoparticles, dye-sensitized metal oxide solar cells, electron transfer processes, heterogeneous catalysis, and water and hydrogen bonding phenomena. We thereby apply quantum-chemical computations and molecular-dynamics simulations using national supercomputer facilities to address these fundamental issues in surface science and atmospheric chemistry.

Nanochemistry. When semiconductor materials are scaled down to nanometer size, many interesting phenomena of quantum-mechanical origin occur. Such nanoparticles will exhibit unique behaviors. We model crystallites of materials such as ZnO, TiO₂, ZrO₂ and Gd₂O₃ and quantum dots of GaN, which are of interest in applications ranging from nanomedicine to optoelectronics. In particular we design novel nanocompounds by functionalizing metal oxide nanoparticles using organic adsorbates. One such example is the dye-sensitized solar cell (DSSC). In this photovoltaic cell organic molecules are chemisorbed at a nanostructured metal-oxide surface (ZnO, TiO₂), where they act as antenna that extend the range of photon wavelengths that can be absorbed from the sunlight. The computations can explain the function of such nanosized systems.

Reactions at solid surfaces. Catalytic reaction mechanisms at crystalline surfaces are important in many processes. In a current project we explore heterogeneous catalysis for carbon dioxide-to-methanol conversion using mixed metal and metal-oxide surfaces (Cu/ZrO₂). This is a KA W-funded project in collaboration with Profs. Ulf Helmersson at Plasma physics, Magnus Odén at Nanostructured materials, Per-Olov Käll and Assoc. Prof. Fredrik Söderlind at Inorganic chemistry. In an ongoing project together with Assoc. Prof. Henrik Pedersen at Inorganic chemistry and Prof. Erik Janzén, Assoc. Profs. Örjan Danielsson and Olle Kordina at Semi-conductor materials we investigate reaction mechanisms in chemical vapor deposition (CVD) processes by computational-chemistry methods.

In addition investigations are being conducted on gas sensor technology in collaboration with Prof. Anita Lloyd-Spetz at Applied physics. Examples of sensors studied are SO₂ sensors using Pt/SiO₂ devices and NH₃ sensors based on RuO₂.

Method development: programs for the calculation of phase diagrams and kinetics based on quantum-chemical data are being created, as well as ab initio MD methods that are useful for elucidating the mechanisms of surface-catalyzed reactions.
Inorganic Chemistry

STAFF
Professor Em: Per-Olov Käll
Assoc. profs: Henrik Pedersen, Fredrik Söderlind

ACTIVITIES
The research in inorganic chemistry at IFM is divided into two research themes: Chemical Vapor Deposition and Applied Nanochemistry. Both themes focuses on synthesis of solid state materials by chemical vapor deposition synthesis of thin films of mainly electronic materials, e.g. BN, B, C and SiC; and by colloidal synthesis of various metal and metal oxide nanoparticles, e.g. ZnO, CuO, ZrO2 and Cu for catalytic and gas sensing applications. The projects are pronounced interdisciplinary and performed in collaboration between chemistry (inorganic chemistry, physical chemistry) and materials physics at IFM.

Chemical Vapor Deposition
Neutron detectors based on the isotope 10B instead of 3He has been suggested by the European Spallation Source (ESS), to overcome the very limited availability of 3He. 10B4C was chosen as the thin film material instead of pure 10B due to its high resistance towards oxidation and wear. In this project, low temperature CVD processes, both thermally activated and plasma enhanced, are developed for deposition of boron carbide films on aluminum blades. Since aluminum is the substrate material, there is an upper temperature limit of 600 °C for the processes, also the use of BCl3 as boron precursor is prohibited by the aluminum. In this project is instead various organoboranes used as single precursors for both boron and carbon.

This project is funded by KAW and done in close collaboration with Prof. Jens Birch at Thin Film Physics and with ESS

Boron nitride (BN) is envisioned to be an excellent material for several electronic applications and can form compounds with either sp3-hybridized or sp2-hybridized B-N bonds. Growth of epitaxial films of sp2-BN presents a great scientific challenge. The CVD research on sp2-BN focuses on fundamental understanding of the growth chemistry for epitaxial growth of sp2-BN to enable BN based electronics. The project is funded by VR and SSF and done in close collaboration with Prof. Anne Henry at Thin Film Physics.

Silicon carbide (SiC) is, apart from being a hard material, a semiconductor material with excellent material properties making it a highly attractive material for electronic devices for high-power, high-frequency and high temperature applications. The current research project on CVD of SiC, funded by KAW, VR and SSF, done in close collaboration with Prof. Erik Janzén at Semiconductor Materials, is focused on developing new CVD chemistry for growth of isotopically pure 28Si2C.

High power pulsed PECVD (HiPP-PECVD) is developed in close collaboration with Dr. Daniel Lundin at Universite Paris-Sud. The research is focused on understanding the plasma chemistry as well as fundamental deposition chemistry in the highly ionized plasma characteristic for HiPP-PECVD.

Applied Nanochemistry
Semiconducting oxide nanoparticles, e.g. ZnO, have shown promising properties as sensing material in gas sensing studies of, e.g., of O₂, NH₃, NOx, CO, H₂. 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. So far, the metal Ir and Pt have shown reasonably good sensing properties for MeOH at elevated temperatures.

Catalytic hydrogenation of CO₂ in the formation of energy rich hydrocarbons, e.g., methanol or dimethyl ether aims at experimental and theoretical studies of the mechanistic catalytic processes involved in the reactions between H₂ and CO₂ in the formation of MeOH or Me₂O (Fig IX below). Although the overall chemistry for these reactions now appears rather well controlled, there is a considerable lack of understanding as to the mechanistic details, in particular regarding the interactions between the surfaces of the solid catalysts and the molecular gas species. A recently purchased high pressure reactor (autoclave) and a combined GC-MS are used for experimental testing of prepared catalysts. Typical reaction conditions are 50 bar and 250 °C. The project is carried out in collaboration with Profs. Magnus Odén at Nanostructered materials, Ulf Helmersson at Plasma & Coatings physics, and Lars Ojamäe at Physical chemistry and is funded by KAW and VR.
Analytical Chemistry

STAFF

Professor: Elke Schweda
Associate professor: Johan Dahlén

Glycoanalysis Research in Analytical Chemistry is focused on analytical carbohydrate chemistry and structures of biologically active carbohydrates from pathogenic bacteria. Of particular interest are the exclusively human pathogen non-typeable Haemophilus influenzae (NTHi) and Campylobacter which is one of the leading causes of bacterial food borne gastroenteritis worldwide. NTHi causes otitis media and both acute and chronic lower respiratory tract infections in small children. The potential of both NTHi and Campylobacter 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.

Designer drugs Collaboration with Swedish National Laboratory of Forensic Science – SKL regarding the analysis of designer drugs has been initiated. A large number of new designer drugs appears on the market every year and the abuse of such substances is steadily increasing. Compound groups in focus are synthetic cannabinoids and cathinones. Reference material of target substances within these two categories has been synthesized. The capabilities of GC-MS and LC-MS for the analysis of these substances are evaluated. Sample preparation, chromatographic separation and identification are also considered.

Highlights

I. Edvin Erdtman joined the group of physical chemistry as research engineer in September 2014. He investigates heterogeneous chemical reactions at surfaces, in particular chemical sensors for NH₃ detection using RuO₂ materials.

II. The determination of the composition of natural gas hydrates (or ice clathrates) by means of vibrational spectroscopy has been aided and given a theoretical foundation by quantum-chemical computational studies, where the spectral patterns of different crystal phases and of the hydrocarbon guest molecules have been mapped out.


III. Plasma chemistry gets a boost from pulsed power: The plasma state is a chemical playground where free electrons and ions open up new reaction pathways at low temperatures. This enables thin film deposition on sensitive materials such as integrated circuit boards. We recently presented a high power pulsed plasma enhanced chemical vapor deposition, which use plasmas several thousand times more electron rich than conventional plasma enhanced chemical vapor deposition. By using carbon films deposited from acetylene as model system, we now show that more film is deposited from the same amount of acetylene and power when the power is delivered as high power pulses. The improved efficiency is attributed to a more efficient plasma chemistry due to the increased number of electrons. J. Vac. Sci. Technol. A 32, 030602 (2014)
IV. Incorporate Chemical Vapor Deposition in teaching:
The complexity and prohibitive cost of CVD equipment makes it seldom available for undergraduate chemistry students. A simple CVD experiment designed to give hands-on experience using common chemical laboratory equipment is outlined in a paper in Journal of Chemical Education. In the experiment, crystalline thin films of titanium nitride (TiN) are deposited using titanium tetrachloride, hydrogen, and nitrogen gas in an experimental setup based on a tube furnace and common safety flasks. J. Chem. Edu. 91, 1495 (2014)

V. CVD of high quality electronic grade SiC using methane as carbon source: Methane is hardly ever used for growing silicon carbide, but it is interesting to study to shed light on the differences in gas phase reactions using different hydrocarbons and the differences in surface reactions of the specie that reach the surface. We observe that methane plays a considerable role for the growth of silicon carbide and it has a much higher probability to stick to the surface than previously believed. We also show that high quality layers may be grown using methane if the carbon to silicon ratio is carefully tuned. J. Cryst. Growth 390, 24 (2014)

VI. Epitaxial growth of rhombohedral boron nitride (r-BN) on SiC: CVD of epitaxial r-BN on SiC was demonstrated using triethyl boron and ammonia as precursors. From X-ray diffraction and transmission electron microscopy, we find that the optimal growth temperature for epitaxial r-BN on the Si-face of the SiC substrates is 1500 °C at a N/B ratio of 642 and silicon needs to be present not only in the gas mixture during deposition but also on the substrate surface. Such conditions result in the growth of films with a c-axis identical to that of the bulk material and a thickness of 200 nm, which is promising for the development of BN films for electronic applications. CrystEngComm 16, 5430 (2014)

VII. Rozalyn Simon successfully defended her PhD-thesis: Anionic oligothiophenes – Optical tools for multimodal fluorescent assignment of protein aggregates.
   Sara Helander successfully defended her PhD thesis: Structural biology of transcriptional regulation in c-Myc network
   Linda Helmfors successfully defended her PhD thesis: Understanding the dual nature of lysozyme: part villain-part hero A drosophila melanogaster model of lysozyme amyloidosis
   Daniel Sjölander successfully defended his PhD-thesis: “Luminescent molecular recognition of pathognomic and ageing associated aggregates”

VIII. The core facility ProLink was initiated to ensure maintenance of our versatile high quality biophysical machine park and open the facility also for external users
SCIENTIFIC BRANCH OF
MATERIAL PHYSICS
General Information

Research Divisions and Professors

Functional Electronic Materials: Weimin Chen (Head), Irina Buyanova

Nanostructured materials: Magnus Odén (Head)

Nanoscale Engineering Division: Kostas Sarakinos (Head)

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

Semiconductor Materials: Erik Janzén (Head), Peder Bergman, Per-Olof Holtz, Leif Johansson (Emeritus), Einar Sveinbjörnsson (Adjunct Prof.), Nguyen Tien Son, 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, Leave in absence SSF), Jens Birch (Acting Head), Michel Barsoum (Guest Prof., Drexel Univ.), Esteban Broitman (Guest Prof. Carnegie-Mellon), Joseph E Greene (Guest Prof., Univ. Illinois) Anne Henry, Ivan Petrov (Guest Prof., Univ. Illinois)

STEERING COMMITTEE

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

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 Project Bridging the THz-gap (Janzén, Main applicant: Zirath at Chalmers)
- KAW Scholar Grant (Hultman)
- KAW Academy Fellow (Rosén)
- KAW Designed Nanoparticles by Pulsed Plas-mas (Helmersson et al.)
- ESF Epitaxial Graphene EPGRAT (Janzén et al)
- EDA/FMV GaN HEMT MANGA (Janzén et al.)
- VR Linnaeus Center LiLi-NFM (Hultman et al.)
- VR/RÅC 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 Synergy Grant FUNCASE (Hultman et al.)
- SSF project: SiC – the Material for Energy-Saving Power Electronics (Janzén et al.)
- The Linköping Center for Nanoscience & Nano-technology CeNano (Kaja Uvdal, 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 about 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 modeling 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 tech-niques 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 tech-niques. Collaboration with foreign laboratories is typical for all research groups; in fact most published papers have international co-authors.

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. Graphensic AB is a spin-off company being the first European company on epitaxial graphene. Another spin-off company, Cyclops AB, develops a novel SiC epitaxial tool. In 2014, two new companies were formed, Classic WBG Semiconductors AB, which will provide ni-tride based HEMT structures, and Polar Light Technologies AB, for the development of polarized light sources.

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

Several patent applications were filed in 2014.

EDUCATION

In 2014, 17 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 (>30 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.

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

**SUMMARY OF ACTIVITIES**

We conduct scientific research on electronic, magnetic and optical properties of semiconductor materials and nanostructures. The materials systems under study in 2014 include: (i) advanced spintronic materials based on III-V semiconductors; (ii) ZnO-based materials and nanostructures; (iii) self-assembled In(Ga)As/GaAs quantum dots (QDs) and QD molecular structures; (iv) dilute nitrides and dilute bismides; and (v) GaP/GaNP and GaAs/GaNAs 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 understanding of the limiting factors in the efficiency of the defect-engineered spin filtering, spin amplification and spin detection at room-temperature.

In the area of ZnO-based materials, several topics were addressed. These include: (i) spin dynamics of a new class of isoelectronic bound excitons; (ii) optimization of defect-mediated energy upconversion processes in bulk and nanostructured ZnO and (iii) understanding the impact of intrinsic defects and unintentional contaminants on n- and p-type doping efficiency.

We have conducted detailed studies of spin-dependent properties of self-assembled InGaAs/GaAs QDs. Special attention was paid to understanding the physical processes of spin injection, spin relaxation and spin detection. We have also studied effect of geometrical arrangements of QD molecular structures such as double QDs, QD clusters and quantum rings on exciton fine-structure splitting, which is relevant to applications utilizing photon-pair entanglement and electron spins.

We have also continued our research activities on optical and structural properties of dilute nitride-based NWs. In the case of GaP/GaNP core/shell structures, the main focus was on optimization of both material quality and structural design to improve radiative efficiency and energy upconversion processes. We have also examined potential of these structures as polarized nanoscale light emitters. Activities related to GaAs/GaNAs core/shell NW structures were mainly devoted to material characterization during 2014.

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.

**PH.D. THESES**

- Yuttapoom Puttisong: “Room-temperature defect-engineered spin functionalities in Ga(In)NAs alloys”.

**LIC. THESES**

- Stanislav Filippov: “Optical properties of novel semiconductor nanostructures”.

**HIGHLIGHTS**

- On the origin of strong photoluminescence polarization in GaNP nanowires [Nano Lett. 14, 193102 (2014)]

In this work we demonstrate that alloying with nitrogen allows one to achieve strong polarization of light emission in individual GaNP and GaP/GaNP core/shell nanowires, which is perpendicular to the wire axis even in zinc blende nanowires of various diameters. The polarization anisotropy can be retained up to room temperature. The observed polarization property is attributed to strong anisotropy of N-related centers responsible for the emission. Our findings therefore show that defect engineering via alloying with nitrogen provides an additional degree of freedom to tailor the polarization anisotropy of III-V nanowires, which is advantageous for their applications as nanoscale emitters of polarized light.

**Energy upconversion in GaP/GaNP core/shell nanowires for enhanced near-infrared light harvesting [Small 10, 4403 (2014)]**

This work shows that though the bandgap energies of GaNP alloys lie within the visible spectral range, coaxial GaNP NWs grown on Si substrates can harvest infrared light utilizing energy upconversion. This energy upconversion can be monitored via anti-Stokes near-band-edge photoluminescence (PL) from GaNP, visible even from a single NW. The dominant process responsible for this effect is identified as being due to two-step two-photon absorption (TS-TPA) via a deep level lying at about 1.28 eV above the valence band. The formation of the
corresponding defect is promoted by N presence. The revealed upconversion process can boost efficiency of harvesting solar energy in GaNP NWs, beneficial for applications of this novel material system in third-generation photovoltaic devices.

![Spectra of upconverted PL emission](image1)

Fig. 2 Spectra of upconverted PL emission (left) and its excitation (right), together with a schematic picture of the energy upconversion process.


In this work we employ electron paramagnetic resonance (EPR) to investigate interactions between the shallow Al$_{2n}$ donor and intrinsic defects that were introduced in ZnO using electron irradiation with variable energies. We unambiguously identify the Aluminum – Zinc vacancy (Al$_{2n}$-V$_{Zn}$) complex as a dominant defect in Al-containing n-type ZnO after electron irradiation with energies above 0.8 MeV. It acts as a deep acceptor with the (0/-) energy level located at ~ 1 eV above the valence band. Such complex is concluded to be a defect of crucial and general importance that limits the n-type doping efficiency by complex formation with donors, thereby literally removing the donors, as well as by charge compensation.

![Atomic structure of the Al$_{2n}$-V$_{Zn}$ complex](image2)

Fig. 3 Atomic structure of the Al$_{2n}$-V$_{Zn}$ complex.

![Spectra of InGaAs/GaAs QDs](image3)

Fig. 4 (a) AFM image of the studied In$_{0.5}$Ga$_{0.5}$As/GaAs QDs. (b) PL spectrum from the QD ensemble at 10 K. (c) PL polarization spectra of the QDs at 10 K as a function of optical excitation power under $\sigma^+$ and $\sigma^-$ excitation.

COLLABORATIONS

We have active scientific cooperation with over 20 internation.

Anomalous spectral dependence of optical polarization and its impact on spin detection in InGaAs/GaAs quantum dots [Appl. Phys. Lett. 105, 132106 (2014)]

We show that circularly polarized emission light from InGaAs/GaAs QD ensembles under optical spin injection from an adjacent GaAs layer can switch its helicity depending on emission wavelengths and optical excitation density. We attribute this anomalous behavior to simultaneous contributions from both positive and negative trions and a lower number of photo-excited holes than electrons being injected into the QDs due to trapping of holes at ionized acceptors and a lower hole mobility. Our results call for caution in reading out electron spin polarization by optical polarization of the QD ensembles and also provide a guideline in improving efficiency of spin light-emitting devices that utilize QDs.
Nanoscale Engineering

STAFF

Associate Professor: Kostas Sarakinos
Post doctor: Daniel Magnfält
PhD students: Viktor Elofsson, Bo Lü
M.Sc. students: Laurent Souqui, Claudia Schnitter
Administrative staff: Therese Dannetun

Associated members: Peter Münger (Associate Professor, Theoretical Physics, IFM), Robert Boyd (Senior Research Engineer, Plasma & Coatings Physics, IFM), Sankara Pillay (Research Engineer, IFM)

ACTIVITY

The Nanoscale Engineering Division was founded in October 2014. Our research aims at understanding and utilizing the complex interplay between materials chemistry, atomic arrangement and physical attributes as a tool to design and create new thin film materials in an atom-by-atom fashion. Our research strategy entails the combined use of:

(i) In situ probes for monitoring microstructural evolution during thin film growth from the vapor phase.

(ii) Stochastic and deterministic growth simulations to understand atomistic processes that determine self-organization processes at the nanoscale.

(iii) Ex situ structural characterization techniques to establish the relationships between synthesis conditions, structure and other physical properties.

An account of our activities during 2014 (partially as part of the Plasma and Coatings Physics Division, LiU) is presented below.

SELECTED RESEARCH HIGHLIGHTS

Growth dynamics

A kinetic Monte Carlo (kMC) code has been developed for the purpose of modeling three-dimensional film growth on a two-dimensional substrate during either continuous or pulsed vapor deposition. It was developed to study the growth mechanisms of noble metals on amorphous insulating surfaces such as silver (Ag) on silicon dioxide (SiO₂, glass). The results of this code have been used in the formulation of an analytical framework that predicts the combination of material and process parameters required to suppress island coalescence, effectively achieving a coalescence-free growth regime. Our analytical framework for continuous vapor deposition was verified against kMC simulations using the code developed here as well as against experimental results from Ag grown on SiO₂ (B. Lü et al., Appl. Phys. Lett. 105, 163107 (2014)). The existence of a coalescence-free growth regime for the case of pulsed vapor deposition was also found and reported (V. Elofsson et al., J. Appl. Phys. 116, 044302 (2014)) and the analytical framework has now been extended to also apply for pulsed vapor fluxes (B. Lü et al., submitted). Our findings open up possibilities to measure the substrate diffusivity of metals on insulator surfaces as well as to tune deposition conditions with enhanced control of the thin film morphology. The continuation of this project involves both applying the theory derived thus far to find yet unknown material properties as well as further development of the kMC code.

Intrinsic stress generation in thin films

A systematic investigation of the causes of intrinsic stresses in sputter deposited refractory thin films has been initiated in collaboration with Profs. G. Abadias (University of Poitiers) and E. Chason (Brown University). Stress data were acquired in situ during film growth experiments where the deposition rate, energetic bombardment and grain size were varied independently. The stress data is currently being analyzed in context of an analytical model in order to discern and understand the fundamental mechanisms affecting the intrinsic stress generation in thin films.

Fig. 1. Snapshots over time from a simulation of the sequential deposition of two metals (grey and yellow atoms) growing in a 3D fashion, as they would on an insulator.

Fig. 2. Intrinsic film stress magnitude dependence on deposition rate and working pressure (pw).
Double in-plane alignment

Biaxially textured thin films consist of grains that are preferentially aligned both out-of-plane and in-plane. For certain materials, two in-plane alignments have been predicted to concurrently evolve in the film; however, experimentally only a single in-plane alignment has been observed. In our work we have shown that the commonly accepted model used to describe the formation of the in-plane alignment overlooks processes related to the development of the out-of-plane alignment. By eliminating the latter processes and growing films that are consistent with the main assumptions of the model we have been able to experimentally verify the existence of biaxially textured Cr films that exhibit a double in-plane alignment. Our findings thus pave the way towards more accurate theoretical descriptions and hence knowledge-based control of microstructure evolution in biaxially textured thin films. (V. Elofsson et al., Appl. Phys. Lett. 105, 233113 (2014)).

Fig. 3. 3D representation of the Cr (200) pole figure indicating the two inplane alignments.

Collaboration

- Prof. Gregory Abadias, University of Poitiers, France
- Dr. Bärbel Krause, Karlsruhe Institute of Technology, Germany
- Prof. Eric. Chason, Brown University, USA
- Prof. Panos Patsalas and Dr. Spiros Kassavetis, Aristotle School of Technology, Greece
- Dr. Nikos Kalfagiannis and Prof. Demos Koutsogeorgis, Uppsala Trend University, UK
- Dr. Vassilios Kapaklis and Prof. Björgvin Hjövarsson, Uppsala University, Sweden

Teaching

The division has during the year been responsible for the undergraduate course TFYA41 Thin film physics.

Nanostructured Materials

Staff

Professor: Magnus Odén
Assistant professors: Naureen Ghafoor, Mats Johansson Jöseaar, Fredrik Söderlind
Post doctors: Emma Björk, Klara Grönhagen, Peter Måkie, Lina Rogström, Jianjiang Zhu
Administrative staff: Therese Dannetun

General Information

The scientific aim of the Nanostructured Materials division conforms to the material science paradigm: understanding of the synthesis, microstructure evolution, and material properties of nanostructured materials of industrial interest. The group 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. Since then, the division has added the project X-cut supported by VR and in 2013 the KA W-financed program Designed nano particles (extended in 2014) and two EU-financed projects: MC2 and SUMA2. Naturally most of the group’s research activities are related to these centers and programs.

Research Programs

Hard Coatings

Nanostructured hard coatings can be used as protective layers for e.g. cutting tools in order to extend the cutting inserts life time. We focus on understanding the behavior of materials during severe condition such that the next generation of hard coatings can be design for better wear protection. The research is performed both experimentally and by theoretical simulations.

Mesoporous Materials and Catalysis:

Mesoporous materials have pores in the size range of 2-50 nm, and large available surfaces (500-1000 m²/g). They are used in applications such as catalysis, drug delivery, and templating of nanoparticles. In Nanostructured Materials, we focus on how the process parameters affect the morphology and pore size of both mesoporous silica particles and films. Also, doping of the silica structure is performed, and the material is used as a template for nanoparticle growth for catalytic applications. The catalytic reactions are studied in a reactor as well as with in-situ FTIR and chemisorption.


**Engineering Materials:**

Aluminum alloys used as either cast automotive engine blocks or heat exchangers are studied. The influence of small (ppm-level) additions of alloying elements on the microstructure evolution during both solidification and brazing is of special interest.

**SCIENTIFIC HIGHLIGHTS**

- In arc evaporated TiCrAlN hard coatings, a Cr-concentration of around 9% plays a key role for the stability of the cubic structure during spinodal decomposition at elevated temperature.

![Fig. 1. Z-contrast (S)TEM micrographs of a TiCrAlN coating annealed at 1100 °C. The cubic TiCr-enriched phase is semi-coherent with the hexagonal Al-enriched phase.](image)

- A new computational method was developed to accurately calculate the Gibbs free energy and thermodynamic properties for random alloys.
- Phase diagrams for TiAIN and AlN was obtained by theoretical calculations including vibrational contribution and thermal expansions.

![Fig. 2. Atom probe measurement show a 3-D structure of arc evaporated TiAIN coating, with capability of providing insights in the phase transformation paths during annealing.](image)

- Magnetron sputtered TiN/Zr0.45Al0.55N coating shows high hardness (34 GPa) at elevated temperature due to its non-isostuctural coherent interfaces between w-AlN rich and C-TiN rich domains.
- In-situ x-ray scattering experiments show that arc evaporated h-ZrAIN coating decomposes during annealing into c-ZrN and h-(Zr)AIN, resulting in nano-sized layers with 2nm periods.

![Fig. 3. Z-contrast STEM and HR-TEM micrographs of the decomposed structure of a ZrA1N coating.](image)

- Successful synthesis of monocrystalline Zr nanoparticles using pulsed plasma.
- High methanol and DME yields when Zr-doped mesoporous silica with Cu nanoparticles was used as a catalyst yield in CO₂ hydrogenation.
- First in-situ FTIR studies of CO₂ hydrogenation in doped mesoporous silica.

![Fig. 4. Successful deposition of CuO nanoparticles on ZnO nanorods using wet chemical synthesis.](image)

**COLLABORATIONS**

The division has strong collaborations both with national and international research groups, as well as with several groups within LiU. Additionally, Nanostructured materials works in close collaboration with industrial partners, including Sandvik Coromant, SECO Tools, Ionbond Sweden and Plansee material composite, and with the division’s spin off company Nanolith Sverige AB.

**OTHER HIGHLIGHTS**

- Two PhDs graduated:
  - Rikard Forsén: Multicomponent Alloying for Improved Hard Coatings
  - Niklas Norrby: Microstructural evolution of TiAIN hard coatings at elevated pressures and temperatures
- Two licentiates defended:
  - Robert Pilemalm: TiAIN-based Coatings at High Pressures and Temperatures
  - Kumar Yalamanchili: ZrN based Nanostructured Hard Coatings: Structure-Property Relationship
- New graduate course: “Transition metal nitride and carbide thin films” developed and given by Naureen Ghafoor and Lina Rogström.
INTRODUCTION

We are an inventive group at the forefront of materials synthesis using advanced plasma techniques. Our goal is to address major challenges facing contemporary materials science and technology. Through a combination of experimental and theoretical tools we seek to understand the process-plasma-material interaction and to gain and exploit our unique insight.

SCIENTIFIC HIGHLIGHTS IN 2014

Nanoparticles Generated by Pulsed Plasma

The division has pioneered the production of nanoparticles via pulsed plasma, in appreciation of which a KAW research project to develop this technology has been awarded. This has led to novel nanoparticles with potential applications including efficient light generation via large area polymeric sources, conversion of CO₂ into energy, enhanced contrast medical imaging and highly selective and sensitive gas sensors to detect volatile organic compounds. In 2014 we demonstrated the versatility of this method as highlighted here.

A unique structure consisting of nanoparticle fibrils decorat- ing nanorods, giving them the appearance of marine coral, have been produced (Fig. 1). These structures have significantly higher exposed surface area compared to a simple coating of nanoparticles. This makes them perfect for catalytic applica- tions, to be explored in the next part of the project. A manuscript further describing our findings is being prepared for publication.

Fig 1: ‘Nanocoral’; unique formation of nanoparticles on nanorods.

Having effective control over the size of nanoparticles during production is one of the key parameters in exploiting their properties. Our process can currently control the size of the particles between 5 nm to 100 nm and we are working to expand this range further. High resolution imaging (Fig 2) also reveals the quality of the particles which are completely crystalline, have no defects and a well-defined oxide layer.

Fig 2: left and inset, Fe nanoparticles. Right, High resolution image reveals the atomic structure of the particle. All images taken at same magnification as indicated by the scale bar.

It was found that by varying experimental conditions, different phases of Titanium Oxide could be formed in a controlled manner (see Fig. 3). The experiments also indicated that oxygen acts as a nucleation seed and its excess can possibly influence the diffusion properties of adatoms deposited on the surface of a nanoparticle, leading to a polycrystalline-structure.

One way to increase nanoparticle production efficiency is to create a geometry where the diffusion losses are reduced. We designed a hollow cathode prototype to test this principle; based on a linear configuration. The geometry also makes the target (cathode) material easier to replace after erosion. We have successfully ignited this cathode (see Fig. 4) and have multiple experiments planned, e.g., testing an array of parallel hollow cathode slits.

Fig 3: X-ray diffraction spectra for reactive synthesis of titanium oxide nanoparticles showing the phase content as a function of the oxygen flow.

Fig 4: Hollow cathode prototype.
**High Power Impulse Magnetron Sputtering (HiPIMS)**

The ability to control the sputtered flux of metal ions has been demonstrated. HfN-thin films can be used as a diffusion barrier against Cu. However, bombardment of ions from the process gas (normally Argon) often introduces defects. In this project, we are selectively using metal ion bombardment. During the pulsed sputtering that occurs in HiPIMS both gas and metal ions are created, but they arrive at the substrate at different times with process gas ions first. Utilizing a synchronized substrate bias, we can select the ion species for film bombardment. This could eliminate the effect of process gas ions, producing films with fewer defects.

**COLLABORATIONS**

The division works with research groups across a wide range of disciplines including photovoltaics, biophysics, thin films and theoretical modelling, both domestically and abroad. Commercial exploitation of our findings is achieved by working with industry and through our spin-out companies; TiÅ, Ionautics and PlasmAdvance.

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**Semiconductor Materials**

**STAFF**

**Professors:** Erik Janzén (Head of Division), Peder Bergman, Per Olof Holtz, Leif Johansson (Emeritus), Bo Monemar (Emeritus), Nguyen Tien Son, Einar Sveinbjörnsson, Rositsa Yakimova (Emerita)

**Associate professors (docents):** Vanya Darakchieva, Urban Forsberg, Carl Hemmingsson, Ivan Ivanov, Anelia Kakanakova, Fredrik Karlsson, Olof Kordina, Plamen Paskov, Henrik Pedersen, Mikael Syväjärvi, Chariya Virojanadara, Qamar ul Wahab

**Assistant Professors, Research fellows & Lecturers:** Örjan Danielsson (Guest lecturer), Jawad ul Hassan, Jianwu Sun, Volodymyr Khranovskyy, Gholam Reza Yazdi

**Post doctors:** Chih-Wei Hsu, Sergey Khromov, Philipp Kühne, Houssaine Machhadani, Daniel Nilsson (started July), Ivan Shtepliuk (started Sept.)

**PhD students:** Nerijus Armakavicius (started Oct.), Chamseddine Bouhafs, Ian Booker, Ir-Tai Chen, Martin Eriksson, Andreas Gällström, Tomas Jemson, Valdas Jokubavicius, Robin Karhu, Xun Li, Louise Lilja, Björn Lundqvist, Björn Magnusson, Daniel Nilsson (PhD June), Pontus Stenberg, Pitsiri Sukhaew, Xuan Thang Trinh, Thien Duc Tran, Chao Xie, Milan Yazdanfar (PhD Oct.)

**Administrative/Technical Staff:** Sven Andersson, Roger Carmesten, Ildiko Farkas, Tihomir Iakimov, Rickard Liljedahl, Xinyu Liu, Vallery Stanishev, Kerstin Vestin, Eva Wibom

**Visiting scientists (at least one month stay):** Yulia Bakakina, Inst. of Biophysics, Belarus, Kateryna Shavano-va, Univ. of Life and Environmental Sciences, Ukraine

**Visiting graduate students (at least one month stay):** Frank Mehnke (Technische Univ. Berlin, Germany), Dmitry Sodzel (Inst. of Biophysics, Belarus), Nelya Slyshyk (Univ. of Life and Environmental Sciences, Ukraine), Makiko Suegetsu, (Saitama Univ., Japan), Shakila Bint Reyaz (Uppsala Univ.)

**INTRODUCTION**

The Semiconductor Materials Division develops and investigates materials for novel electronics with the main focus on silicon carbide, (SiC), III-nitrides (GaN, InN, AlN and their alloys) and graphene. The goal is to resolve fundamental and application-motivated issues of interest for Swedish and European industries. The research activities within the division cover a broad spectrum dominated by basic research, mainly funded by Swedish and European agencies, partly with industrial collaboration. There is a strong international cooperation within most research projects.

**Current Research Activities**

- Growth, simulation and characterization of epitaxial films and bulk crystals.
- Investigations of crystal defects and doping.
- Development and studies of nano- and heterostructures
The growth is based on chemical vapor deposition (CVD) or sublimation techniques while the characterization includes surface and interface properties as well as structural-, optical- and transport properties probed by techniques such as photoluminescence spectroscopy, magnetic resonance, DLTS, ellipsometry, XRD, photoelectron spectroscopy and microscopy.

High Frequency and High Power

SiC is a semiconductor material that sustains higher frequencies, powers and temperatures than conventional silicon. This leads to smaller electronics and reduced power loss, with applications in electric power distribution and power electronics in hybrid cars. Significant efforts within the division are devoted to develop high quality SiC for devices. One ambition is to control the involved isotopes and thereby improve its thermal properties.

The III-nitrides is a class of materials that exhibit extremely good high-frequency characteristics, in addition to their outstanding light emitting properties. A project within the division aims to develop the nitride material for high electron mobility transistors, with applications in the next generation high-speed data transmission systems.

The division has recently gained attention also for graphene, in particular for a high temperature fabrication process of graphene on SiC. The exceptionally high carrier mobility in graphene makes it a promising material for new devices operating up to the terahertz frequency range.

Novel Light Sources

The optically efficient III-nitrides have enabled new and energy efficient light sources, such as LED-lamps and blue lasers. Within the division, there is a constant activity for deepening the understanding of the III-nitrides and for improving the material quality in order to further enhance its light emitting performance.

One challenge tackled by the division is to develop a III-nitride based light emitting material for deep ultraviolet lasers. The disinfecting properties of ultraviolet light can be utilized for water cleaning. III-nitride based single-photon emitters are fabricated and investigated for their potential use in quantum information applications. Other optically efficient materials, e.g. zinc oxide (ZnO), are also studied.

SPECIAL EVENTS 2014

Two new spin-out companies were formed from our research activities on silicon carbide and III-nitrides:

**Classic** – In spring 2014, Classic WBG Semiconductors AB was formed. The four founders of Classic all come from the division of Semiconductor Materials, having rich experience and knowledge in growth and characterization of nitrides and SiC materials. Classic is in a highly expansive phase and in 2015 the company will participate in two European projects with the aims (1) to fully exploit the high thermal conductivity of the isotope-pure SiC materials and (2) to be qualified as the European supplier of nitride based HEMT structures.

**Polar Light Technologies AB** – Based on a successful research project on nitride semiconductor quantum dots, a novel method for efficient generation of polarized light has been attained. A Swedish patent was finalized in the end of 2014, while an international patent will be finalized in the beginning of 2015. The concept has potential for applications such as optical interconnects, LCD back lighting and secure communication. For the further development of this concept into future commercialization of the innovation, a spin-off company, Polar Light Technologies AB, was started in Dec 2014.

**Sweden – South Africa exchange program.** Based on a program financed by a VR-Link program, there has been an extensive exchange series involving both junior and senior researchers during the period 2011-2014. For evaluations and conclusions, there has every year been a workshop arranged, every second year in South Africa and every second year in Sweden. During the period of 15-18 June, 2014, there was a final workshop within this VR-Link program, arranged in Karlskrona, attracting around 25 researchers from Linköping University and South African universities.

**Olof Kordina** received his Docent degree in June 2014.

**RESEARCH FUNDING**

The turnover for research in our division was about 55.1 MSEK during the period 140101-141231, including depreciation costs for equipment. The major part of this budget comes from external sources. The faculty support for research was about 7 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, Swedish Innovation Agency (VINNOVA), European Defense 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.

**SELECTED RESEARCH PROJECTS**

**Major National Projects**

**Isotope project** – A major part of the KAW grant 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 spectral linewidth, 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. The instrument for precise measurements of the thermal conductivity is under development, to be delivered in the spring 2015. A new reactor designed to grow the isotope-enriched material using any sources was installed during 2014. We have investigated suitable process conditions for SiC epitaxy from SiF4. Good crystal quality has successfully been achieved, however a more fundamental understanding of the growth behavior is still lacking. This work continues combining experimental and modeling efforts. PI: E. Janzén.

**The SSF project SiC** – the Material for Energy-Saving Power Electronics started in 2012 and is focused 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) Characterization 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. A new carrier lifetime limiting defect, RB1, has been identified to be related to iron contamination. Iron is believed to originate from corrosion of reactor parts when using chlorinated chemistry. To further increase the understanding of the Cl-based epitaxy, growth using another halogen species was investigated, namely Bromine. By comparing the two different chemistries, both experimentally and theoretically, new insights have been achieved e.g. regarding important growth species. PI: E. Janzén.

**Bridging the terahertz gap** – In this project, financed by KAW, the Semiconductor Materials Division is working in close collaboration with Chalmers University in Gothenburg and KTH in Stockholm to develop new electronics for telecommunication in the terahertz frequency range. Excellent materials for the active area of such devices are indium nitride (InN) or indium rich indium gallium nitride (InGaN). The Semiconductor Materials Division is here focusing on understanding and developing the synthesis of very thin layers of InN and InGaN by chemical vapor deposition. The challenge lies in the high tendency for the indium atoms to desorb from the surface, which means that the materials synthesis must be performed at a low temperature. One approach for this is to steer the synthesis chemistry from the gas phase to the surface by using an atomic layer deposition approach where the In and N precursor molecules are sequentially pulsed into the reactor to saturate the surface with either In or N atoms. The surface chemistry of the In saturated surface can break down the N precursor at low temperature which enables a low overall synthesis temperature. Partner: E. Janzén.

**European projects**

**Manga** is an initiative to develop nitride-based technology. The Manga project is a European large-scale project to develop GaN HEMT structures. Our contribution is to investigate heat transport in a HEMT device and optimize nucleation layer to improve heat dissipation of the HEMT device. This is a very important part since it improves the reliability of the transistor. Parallel to Manga, additional minor national programs have been added. Part of these programs involve development of carbon doping using both residual and intentional carbon doping. Carbon doping of GaN is an important step to obtain semi insulating GaN buffer layer in the HEMT device. However, carbon can also cause trapping phenomena, which have been investigated within these national programs. PI: E. Janzén.

**The Graphene flagship** started in October 2013, involving 126 academic and industrial research groups in 17 European countries with an initial 30-month-budget of 54 million euro. We are partner in this project with focus on sublimation growth of graphene on SiC. This initiative will help us to implement our ideas on how to scale up the production of graphene. PI: R. Yakimova

**GraphOhm** is an ongoing EU Joint Research Project that started June 2013 on Quantum resistance metrology based on graphene. Our contribution is epitaxial graphene on SiC. PI: R. Yakimova.

We have also been providers of graphene on SiC in the **Nano-RF** project, which is an ongoing collaboration on Carbon Based Smart Systems For wireless applications. Partner: R. Yakimova.

During 2014, we participated in two projects within the Marie Curie Actions Research Fellowship Program: **NetFiSiC** is a project on interfaces on SiC that has been funding one PhD student for researching graphene on SiC since 2012. **BIOSENSORS-AGRICULT** is a project on developing nano-technology-based biosensors for agriculture with partners from France, Latvia, Belarus and Ukraine. 6 researchers where involved in the staff exchange scheme of IFM during 2014. Partner: R. Yakimova.

**Other Major International Projects**

**LG-Innotek** – 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 chlorinated epitaxial process that has been studied here for several years. The project is now in its second phase (year 4-6). The focus is on reducing the density of structural defects that are harmful to the device performance and increase and control the carrier lifetime of the material, which is an essential part in the fabrication of bipolar devices. The lifetime of the carriers is strongly correlated with various defects in the material. The dominating defect in as-grown material is the carbon vacancy and it is manifest in the epitaxial material at different concentrations depending on growth conditions. We are continuing to map out the correlation between the carrier lifetime with the growth conditions. Ways of improving the
lifetime, such as high temperature oxidation, is also under investigation. For this reason an oxidation furnace has been built for temperatures above 1500 °C.

**PUBLICATIONS**

Research activities in this division during 2014 have produced 65 articles published in well-recognized international journals, 18 conference proceedings papers with peer review as well as one review article and one book chapter. 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 with more than 27500 ISI citations. Details and highlights of the research work as well as updated publication lists are available at our website: www.ifm.liu.se/semicond.

**SELECTED RESEARCH HIGHLIGHTS**

**Single spins in silicon carbide**

Unpaired electrons at an electronic defect in solids possess an intrinsic angular momentum, often called spin. Single spins can be prepared in an arbitrary state and are basic elements for quantum computing where states of spins are used as quantum bits. Leading contenders such as defects in diamond or individual phosphorus dopants in silicon have shown spectacular progress, but either lack established nanotechnology or an efficient spin/photon interface. Silicon carbide (SiC) combines the strength of both systems: it has deep photoluminescence (PL) defects and benefits from mature fabrication techniques. Research teams at Linköping, Takasaki, Stuttgart, Budapest, Beijing and Chicago have successfully designed and fabricated 4H-SiC single crystal samples with the Si vacancy (missing Si atom) or divacancy (missing neighbouring Si and C atoms) at low concentrations so that single defects can be observable in an optical confocal microscope and selectively detected by PL. Overcoming difficulties in control of the charge state of defects and other issues in the detection of weak light emission, the research teams have been able to manipulate and detect single spins in SiC at room temperature (for the Si vacancies) and at cryogenic temperatures (-253 °C for the divacancies), showing long spin coherent times up to 1.2 milliseconds. The demonstrated ability of optically single-spin control at room temperature shows the potential applications of defects in SiC for quantum processors that could operate at ambient conditions and pave the way for integrated spintronics.

▶ D. J. Christle et al., Nature Materials (2014) doi:10.1038/nmat4144; M. Videnmann et al., ibid doi:10.1038/nmat4145

**Graphene on cubic SiC**

We applied a high temperature process to grow graphene on cubic silicon carbide (3C-SiC). No buffer layer was observed for the graphene grown on the (001) plane, as confirmed by low energy electron microscopy (LEEM) and diffraction (LEED). The cubic symmetry of 3C-SiC leads to a lack of spontaneous polarization, as confirmed by the mild n-doping (n = 7.4×10^10 cm^-2) observed in graphene grown on the (111) plane by angle-resolved photoelectron spectroscopy (ARPES). We demonstrated from different aspects that 3C-SiC is a good substrate for growth of epitaxial graphene. The 3C-SiC samples were grown in a well-controlled process for high crystalline quality without foreign polytype inclusions.

▶ P. Hens et al., Carbon 80 823 (2014); S. Mammadov et al., 2D Mater. 1 035003 (2014); V. Jokubavicius et al., Cryst. Growth Des. 14 6514 (2014)

**Assessing properties of mixed crystal structures in thin films**

When grown under non-equilibrium conditions, crystals or thin films of technologically important materials may contain domains with different crystal structures. Here we develop and demonstrate nondestructive structural and optical methods to determine the ratio between different crystal phases and study the free-charge carrier and vibrational properties of mixed-phase films. Our approach allows us to establish the elusive properties of cubic InN.


**Study of Ag-dopants on the structural and optical properties of ZnO nanorods**

Zinc oxide (ZnO) is a semiconductor material promising for optoelectronics due to its efficient light emitting properties. However, the key challenge that must be solved before ZnO can be used as a LED material is to make it so-called p-type. Substitution of some Zn atoms with silver (Ag) was recently proposed as an approach for obtaining p-type ZnO. Here we investigate the structural and optical properties of ZnO nanorods doped with Ag atoms. We demonstrate that Ag promotes the generation of crystal defects and significantly modifies the optical spectrum of ZnO. These results can be of high importance for further progress on p-type ZnO.


**Resolving the doping limitations in aluminum gallium nitride**

We achieve better understanding of the complex growth phenomena underlying the deposition of aluminium gallium nitride (AlGaN) alloys and the related doping by silicon (Si). We can grow respective layers of such crystal quality and doping characteristics as to support the study of fundamental material properties of AlGaN. For that, an essential and sophisticated method such as the electron paramagnetic resonance (EPR) is implemented. We can explain the sharp increase of resistivity of Si-doped AlGaN layers with the increase of Al content.

Micropyramid emits antibunched photons in the ultraviolet spectral region

Linearly polarized photons emitted one by one form the basis for novel cryptography methods. Here we demonstrate that the photons emitted from an InGaN quantum dot grown on the apex of a GaN micropyramid exhibit single photon characteristics known as antibunching. Our experiments show that the quantum dot itself is a fast and close to perfect single photon emitter, but a superimposed background signal from the pyramid needs to be eliminated before utilization in polarization-based single photon applications.


High thermal stability quasi-free-standing graphene on silicon carbide through Platinum functionalization

Graphene grown on silicon carbide (SiC) provides solutions for high frequency electronics operating at high temperature. However, a major obstacle is that the electrons are substantially slowed down due to the first carbon layer formed on the SiC. Here we report on quasi-free-standing graphene layers with potentially fast electrons even at very high temperatures (1200°C), achieved by letting Platinum penetrate into the graphene-SiC interface.

▶ C. Xia et al., Carbon 79, 631 (2014)

Resonant ionization of shallow donors in electric field

Semiconductors are non-conductive at low temperatures because the electrons freeze in their lowest energy state at impurities. However, a sudden rise of the conductivity can occur at very high electric fields due to resonant ionization. We discuss this effect using a simplified model of the energy states of donor impurities, and our results are similar to the predictions of more advanced models and in very good agreement with our experiment.


Layer-number determination in graphene on SiC by reflectance mapping

Graphene attracts much attention due to its exceptional properties for future electronics. Growth of graphene on silicon carbide is promising for large-scale device-ready production. A significant parameter characterizing the quality of the grown material is the number of layers. Here we report a simple, handy and affordable optical approach for precise number-of-layers determination of graphene based on the reflected power of a laser beam.

▶ I. G. Ivanov et al., Carbon 77 492 (2014)

Nano-resolution reveals the true nature of graphene

Graphene grown on the basal planes of silicon carbide is considered a most promising route for carbon-based nanoelectronics. Two nonequivalent faces of silicon carbide can be used for this purpose, the carbon-face and the silicon-face. It was claimed that these two faces result in graphene with fundamentally different electronic properties. Here we reveal the actual similarity between graphene layers on the two faces by experiments on a nanometer scale. Moreover, the apparent difference previously seen in standard experiments can now be explained as the collective effect of microscopic grains of graphene formed on the carbon-face.


Plasma chemistry gets a boost from pulsed power

In the plasma state, free electrons and ions open up new low temperature reaction pathways, enabling thin film deposition on sensitive materials such as plastics. We recently presented the concept of high power pulsed plasma enhanced chemical vapor deposition (HiPP-PECVD), which use plasmas thousands of times more electron rich than conventional PECVD. By using carbon films as model system, we now show that more film is deposited from the same amount of acetylene and power when the power is delivered as high power pulses. This is attributed to a more efficient plasma chemistry due to the increased number of electrons.


Please visit www.ifm.liu.se/semicond for details and more highlights.

STUDENT THESES

Doctoral theses

Milan Yazdanfar: Precursors and defect control for halogenated CVD of thick SiC epitaxial layers

Daniel Nilsson: Doping of high-Al-content AlGaN grown by MOCVD

Licentiate theses

Thien Duc Tran: Investigation of deep levels in bulk GaN

Xuan Thang Trinh: Electron Paramagnetic Resonance Studies of Negative-U centers in AlGaN and SiC

Master theses

Fatima Akhtar: Study the effect of ambient conditions on epitaxial graphene

Fang-Wei Chen: Growth of Carbon Nanomaterials on SiC

Bachelor theses

Jimmy Thörnberg: Investigation of Hexagonal GaN Pyramids and InGaN Quantum Dots
TEACHING

The division is very active in teaching and it has responsibility of about 20 undergraduate and graduate courses at IFM.

UNDERGRADUATE & MASTER COURSES OFFERED 2014

- TFFM08 Experimental Physics (Son)
- TFYY51 Engineering Project Y (Forsberg)
- TFYY70 Physics of Cond. Mat. I (Virojanadara)
- TFYA20 Surface Physics (Virojanadara)
- TFYY47 Semiconductor Physics (Karlsson)
- TFYY57 Nanophysics (Paskov)
- TFYA15 Models in Physics (Karlsson)
- TFYY68 Mechanics (Hemmingsson)
- TFYY55 Physics (Bergman)

PHD COURSES OFFERED 2014

- Properties of III-nitride semiconductors (Paskov)
- CAD of scientific use (Kordina)
- Growth perspectives III-V materials (Kakanakova)
- Raman spectroscopy (Ivanov)
- Trends in the periodic chart (Pedersen/Högberg)
- Growth and characterization of ZnO (Khranovskyy)

POPULAR SCIENCE ACTIVITIES

The Semiconductor Materials division arranged a study visit by about 70 junior high school students from Vadstena with help from the Biomolecular and organic electronics division. The students spent 5 hours at IFM, learning about our research and its relation to energy and sustainable development. They participated in lectures about semiconductor growth, energy saving power electronics, graphene and organic solar cells. The youth also visited our research labs with exciting hands-on experiments and demonstrations. The event involved five senior researchers and four PhD students.

Our division also participated with exhibitions and hands-on experiments at LiU’s Popular Science Week, mainly targeting high-school students and teachers. We demonstrated the effects of polarized light in connection to our research on ellipsometry, as well as photoluminescence and III-nitride LEDs linked to our research on optical properties and spectroscopy of semiconductor materials.

Olle Kordina visited Soltorgsgymnasiet in Borlänge and talked about electricity usage and SiC based power electronics. Bo Monemar, Per Olof Holtz and Carl Hemmingsson gave lectures about the Noble Prize in Physics 2014 – a topic strongly related to our research on III-nitrides.
Surface and Semiconductor Physics

STAFF

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

Assistant lecturer: Peter Andersson

Teaching assistant: Maria Pihl

Post-doc: Wei Min Wang, Hafiz Muhammad Sohail

PhD students: Jalil Shah

Adm/Techn. staff: Kerstin Vestin, adm. asst., 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 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 and chemical properties 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 is supported by a grant from the Swedish Research Council (VR) to study the electronic and atomic structure of surfaces, surface alloys, and silicene (Roger Uhrberg).

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) and metal-oxide field effect transistors (MOSFET) for applications in optoelectronics, rf technologies and power-electronics.

Within this field, Wei-Xin Ni is supported by 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.

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 and Nanotechnology: TFYA38 Optoelectronics (Ni), TFYA25 Physics of Condensed Matter, part II (Uhrberg), PhD course: Solid State Physics I (Uhrberg)

HIGHLIGHTS

Figure 1 (a) shows a low energy electron diffraction (LEED) pattern of the Ag/Ge(111) 1/3x1/3 surface which has a two-dimensional (2D) free-electron like band structure. The surface band is partially filled which makes the surface metallic. By introducing a higher order periodicity, one can change the size of the unit cell in reciprocal space and thereby changing the fundamental properties of the electronic structure. An addition of 0.2 ML of Ag onto the surface results in a new reconstruction with a 6x6 periodicity shown by the LEED pattern in Fig. 1 (b). The electronic structure of the Ag/Ge(111)6x6 surface was studied using angle resolved photoelectron spectroscopy (ARPES). In Fig. 1 (c), two dimensional constant energy contours at 0.2 eV below E_F are shown, obtained using a photon energy of 30 eV at RT. There are two circles at the top and the bottom of Fig. 1 (c) which are due to the 2D surface band of the 1/3x1/3 surface. In addition, there are some other weak circles in Fig. 1 (c) which are the result of umklapp scattering due to the new higher order 6x6 periodicity. The effect of the umklapp scattering is schematically illustrated by the red circles (surface band structure) in Fig. 1 (d), where also the 6x6 surface Brillouin zones are illustrated. The overlap of umklapp scattered surface bands, illustrated by the overlapping circles, results in gap openings at the SBZ boundaries transforming the initially metallic surface band structure into a semiconducting one. The complicated pattern of umklapp scattered constant energy contours is schematically illustrated in Fig. 1 (e).

▶ Hafiz M. Sohail, R.I.G. Uhrberg, Surf. Sci. 23-29, 625 (2014);
2) Following the earlier experience and success in fabricating various Si/SiGe-based two- or three-terminal devices using layered or low-dimensional Si/SiGe-heterostructures made by molecular beam epitaxy (MBE), with improved performance in RF- and photonic-applications, the group continues its effort in making high quality Si-based epitaxial structures for advanced device applications. The group has recently focused on studies on the growth kinetics in a low flux regime, in order to enable the controlled growth of Si layers on some silicide or silicon-carbide (SiC) templates, for new devices.

The growth of Si/SiGe on Co1-xNixSi2 is motivated by THz SiGe HBTs, which demand a very low contact resistance. By exposing the silicide surface to a low flux Si beam (in the order of 0.01 Å/sec) at a substrate temperature range of 700-800 °C, the silicide growth template can be cleaned, forming a homogeneous monolayer-scale Si top surface. A defect-free Si layer (≤10 nm) was thereby successfully grown on Co1-xNixSi2 at low temperatures (~350 °C) with a very flat and homogenous interface between Si and silicide layer. The critical thickness of a defect-free Si layer on Co1-xNixSi2 was also determined for the growth below 400 °C, which enabled the successive growth of thicker Si/SiGe heterostructures on the silicide patterns through an oxide window at a desired temperature.

The group has also carried out some research activities aiming at developing the techniques that can produce a dielectric layer on SiC for high electron mobility in the channel region and a high dielectric strength. By investigating the detailed chemical processes involved during the oxidation of SiC, we have tried a new mean to clean and pre-oxidize the carbide surface using UV ozone, followed by PECVD deposition of a SiNy/SiOx double stack, and post-annealing in ambient of oxygen and/or nitrogen. The fabricated SiC-MOS capacitors were characterized by C-V experiments, and the results are summarized in Fig. 2. Different annealing conditions yielded different flat-band voltages, \( V_{\text{FB}} \), in the measured C-V curves. \( V_{\text{FB}} \) can be controlled to be < 1 V with essentially no hysteresis for the sample annealed at 850 °C for 1 hr in oxygen ambient. Furthermore, the dielectric strength of the SiNy/SiOx double stack was measured to be > 5x10^6 V/cm, which is compatible to the thermal SiO2 (10^7 V/cm).

3) The two-dimensional (2D) honeycomb structure of carbon atoms, i.e., graphene, has attracted great attention because of its outstanding electronic properties due to sp2 hybridization and the resulting \( \pi \) band with its linear dispersion and Dirac cone. Inspired by the result from graphene, a lot of effort is now put into the search for other 2D sp2 hybridized materials. As the nearest neighbor to C in group IV, Si is a promising candidate and it is of high interest because of the application potential in Si-based electronic devices. The 2D honeycomb structure of Si, called silicene, has been theoretically studied since the 1980’s. Free-standing silicene is calculated to be stable only in a slightly buckled geometry. In recent experiments, silicene has been synthesized on Ag(111) which is believed to be the best substrate. Different mixes of sp2/sp3 hybridizations on the surface results in different reconstructions of the silicene showing (4×4), (\( \sqrt{3} \times \sqrt{3} \)), (\( \sqrt{7} \times \sqrt{7} \)) or (2\( \sqrt{3} \times 2\sqrt{3} \)) periodicities with respect to the Ag(111) surface lattice. Fig. 3 (a) shows an atomically resolved STM image of the (2\( \sqrt{3} \times 2\sqrt{3} \)) structure. The bright parts show a well-defined (2\( \sqrt{3} \times 2\sqrt{3} \)) order, while the intermediate regions are less ordered. The \( (4 \times 4) \) periodicity shown in Fig. 3 (b) is very well-ordered with just a few vacancies in the regular array of Si atoms. Fig. 3 (c) shows an STM image of the \( (\sqrt{7} \times \sqrt{7}) \) periodicity which is formed by the honeycomb like structure. These surfaces are studied by angle resolved photoemission at MAX-lab in order to determine the electronic structure.
Figure 3. (a) Atomically resolved filled state STM image of a 11.0×16.4 nm² area showing a local (2√3×2√3)R30° honeycomb structure and a long range quasi-regular hexagonal modulation. (b) Filled state STM image of a 13.2×13.2 nm² area showing a (4×4) periodicity. (c) Empty state STM image of a 13.2×13.2 nm² (√13×√13)R13.9° area. All images were obtained at room temperature with a tip bias -1.5 V for (a), (b), and + 1.2 V for (c).

ASSIGNMENTS

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 Universitaet (Prof. G. Bauer, Dr. T. Fromherz), Heriot-Watt University (Prof. C. Pidgeon), National Nano Device Labs in Taiwan (Drs. M.-N. Chang and J.-M. Shieh), Tsinghua University (Dr. D.-G. LiU), Xi-Dian University (Profs. Y. Hao, and Y.M. Zhang). In some projects involving synchrotron radiation we collaborate with Dr. K. Sakamoto, Chiba University, Japan.

Thin Film Physics Division

ORGANIZATION
The Division is organized in six groups based on research leaders and topics:

- **Nano-materials Science** (J. Birch)
- **Materials Design** (J. Rosén)
- **Energy Materials** (P. Eklund)
- **Electron Microscopy of Materials** (P. Persson)
- **Fundamental Science of Thin Films** (G. Greczynski)
- **Functional Materials** (H. Högberg)

BRIEF OVERVIEW
The Thin Film Physics Division conducts 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. Our research concerns design of new multifunctional materials for hard and wear-resistant coatings, energy materials, magnetic materials, electronics, neutron-converting materials for the ESS, wide-bandgap semi-conductors, and more. 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 in applications.

STAFF
**Professors:** Jens Birch (Acting Head of Division, Group Leader), Anne Henry, Esteban Broitman (Guest Prof., Carnegie-Mellon), Michel Barsoum (Guest Prof., Drexel University), Joseph E. Greene (Guest Prof., University of Illinois), Ivan Petrov (Guest Prof., University of Illinois), Lars Hultman (75% leave of absence (CEO SSF))

**Associate Professors:** Johanna Rosén (Deputy Head, Group Leader), Hans Högberg (Deputy Head, Group Leader), Per Eklund (Group Leader), Per Persson (Group Leader), Grzegorz Grezczynski (Group Leader), Valeriu Chirita, Fredrik Eriksson, Jens Jensen, Martin Magnuson, Galia Pozina, Gueorgui Gueorguiev

**Assistant Professors or Lecturers w/o Docent degree:** Björn Alling (Docent), Ching-Lien Hsiao, Per Sandström, Magnus Garbrecht

**Researchers:** Carina Höglund (ESS AB), Jun Lu, Lars-Åke Näslund

**Post Docs:** Axel Flink (Impact Coatings AB, end 2014), Ámi Sigurður Ingason (University of Iceland), Biplab Paul (IIT Kharagpur), Camille Pallier (Univ. Bordeaux), Susann Schmidt (LiU), Jeremy Leroy Schroeder (Purdue University), Oleksiy Voznyi (Ukraine), Igor Zhirkov (Tomsk State University), Davide Sangiovanni (LiU), Hanna Fager (LiU), Justinas Palisaitis (LiU/Jülich), Agne Zukauskaite (LiU, now Fraunhofer Inst. Freiburg)

**PhD Students:** Steffen Senderby (industry PhD stud., DTI, PhD 2014), Hanna Fager (PhD 2014), Martin Dahlqvist (PhD 2014), Olof Tengstrand (PhD 2014), Aurelijus Mockūtie (PhD 2014), Hanna Kindlund, PhD 2014, Agne Zukauskaite (PhD 2014),
Konstantinos Bakoglidis, Mikhail Chubarov (Mihails Cubarovs), Daniel Edström (Licentiate), Annop Ektarawong, David Engberg Mathias Forsberg, Amin Gharavi, Cecilia Goyenola, Joseph Halim (Lic., also at Drexel University, USA), Tuomas Hänninen, Linda Karlsson, Sit Kerdsongpanya (Licentiate), ChungChuan Lai, Ludvig Landälv (industry PhD Student, Sandvik), Mewlude Imam (Yimamu Maiwulidan), Rahele Meshkian, Marlene Mühlbacher also at Leoben Univ., Austria, Andrejs Petruhins (Licentiate), Alexandra Serban, Quanzheng Tao, Lina Tengdelius, (Licentiate), Christopher Tholander (Licentiate), Andreas Thore (Licentiate)

**Administrative and Technical Staff**: Anette Frid (Division Coordinator, from 2014), Kirstin Kahl (Division Coord. (until 2014) AFM Coord.), Malin Wahlberg (Division Coord. (until 2014) Linné C.), Therese Dannetun (FunMat Vinnex Center Coordinator), Thomas Lingefelt (1st Research Engineer), Harri Savimäki (Research Engineer)

**External Research Funding**:
- ERC Advanced Grant (Hultman)
- ERC Starting Grant (Rosén)
- ERC Starting Grant (Eklund)
- VR Distinguished Young Researcher (Rosén)
- SSF Future Research Leaders 5 (Eklund)
- VR International Career Grant (Alling)
- KAW-Scholar (Hultman)
- KAW Academy Fellow (Rosén)
- VR Special Researcher (Persson)
- EU FP7 LifeLongjoints (Högberg)
- Strategic Grant (SFO) in Materials Science, AFM
- SSF Synergy Grant, FunCase
- VR Linnaeus Grant, LiLi-NFM
- Vinnova Excellence Center, FunMat
- VR/RÅC Coordinated Frame Program (Birch)
- 11 VR Project Grants (Pls: Birch, Henry, Bar-soum, Hultman, Rosén, Eklund, Persson, Alling, Hsiao, Pozina, Greene)
- EnergyAgency: Defects physics in GaN (Pozina)
- VR Swedish Research Links (Gueorguiev)
- SSF Korea-Sweden (Henry)
- Eurostars: T-to-Power (Eklund)
- ÅPF: Development of hybrid LEDs (Pozina)
- ÅPF: ScALN (Zukauskaite)
- 5 Carl Trygger grants (Henry, Gueorguiev, Jensen, Magnuson, Schmidt)
- STINT Cluster-assembled materials (Gueorguiev)
- Partner Petra III Swedish Beamline P21 (Birch)
- Partner MAX-IV VERITAS Beamline (Magnuson)
- KAW-Project (Janzén, Abrikosov, Birch, Hultman)

**UNDERGRADUATE COURSES OFFERED**
- TFYA21 Materials Science (Alling)
- TFYA46 CDIO – Biology and Chemistry (Henry)
- TFYA50 CDIO – Computational Physics (Chirita)
- TFYA53 Computational Physics (Chirita)
- TFFM 40 Analytical Methods in Mtrl Sci. (Eriksson)
- TFYY47 Nanotechnology (Birch)
- NFYA04 Nano Scientific Project (Rosén)
- TFYA27 Advanced Project Appl. Phys. (Eklund)
- TFE171 Electrical Measurem. Systems (Sandström)
- TFMT13,16,22 Measurement Technol. (Sandström)
- TFYA65 Physics of Sound (Sandström)
- TSTE05 (IFM part) Electr. & Meas. Tech. (Sandström)

**GRADUATE COURSES OFFERED**
- Synchrotron Radiation (Magnuson)
- Ion Beam Analysis of Condensed Matter (Jensen)
- Fundamentals of Ceramics (Barsoum)
- Nucleation and Growth (Greene, Birch, and Hultman)
- Vacuum Science and Technology (Eklund)
- Electron Microscopy (Persson)
- X-ray Diffraction (Birch and Eriksson)
- Surface Anal. Techn. (Greczynski, Jensen, Sandström)
- Introductory course to SPM (Sandström)
**PHD THESES IN 2014**

Agne Zukauskaite, Hanna Fager, Hanna Kindlund, Steffen Sønderby (industry PhD stud., DTI, PhD 2014), Martin Dahlqvist (PhD 2014), Olof Tengstrand (PhD 2014), Aurelija Mocküte (PhD 2014)

**SPECIAL EVENTS IN 2014**

- Johanna Rosén received VR Distinguished Grant
- Per Eklund received SSF Future Research Leaders
- Per Persson organized the SCANDEM2014 conference in Linköping
- Carina Höglund received the Chester Carlson Award
- Björn Alling received the VR International Career Grant (INCA)
- Agne Zukauskaite received a Junior Group Leader position at the Fraunhofer Institute, Freiburg, Germany (starting Feb. 2015)

**SCIENTIFIC HIGHLIGHTS IN 2014**


At the Swiss Light Source (SLS) we have made a discovery that could be a step to superconductivity at room temperature. Using advanced X-ray spectros-copy we have found that a certain hole-injection configuration is temperature-dependent at the phase transition in the superconductor YBa$_2$Cu$_3$O$_7-x$. M. Magnuson et al Scientific Reports 4, 717 (2014).

We have revealed the structural diversity of carbon fluoride, CF$_x$. C. Goyenola, S. Stafström, S. Schmidt, L. Hultman, J. Phys. Chem.C 118 (2014) 6514–6521

We demonstrated growth of two-dimensional Ti$_4$C$_2$ thin films of the novel class of 2D materials called ‘MXene’. These films exhibit weak localization of charge carriers and thus prove that these materials are genuinely two-dimensional in that there is quantum confinement of charge carriers. Halim....., Eklund, Barsoum, Chem. Mater. 2014, 26, 2974

A novel two step sputtering/annealing method for thin film growth of textured Ca$_3$Co$_4$O$_9$ was invented where a CaO-CoO thin film was deposited by reactive rf-magnetron co-sputtering from Ca and Co targets. Synchrotron-based 2D x-ray diffraction as well as ex-situ annealing experiments and standard lab-based x-ray diffraction analyses reveal the underlying mechanism of thermally activated phase transformation from CaO-CoO phase to the final phase of Ca$_3$Co$_4$O$_9$. B. Paul, ....... J. Birch, P. Eklund, Advanced Electronic Materials, in press.
We developed a novel strategy for low-temperature growth of dense, hard, and stress-free refractory ceramic thin films. The method employs hybrid high-power pulsed and dc magnetron co-sputtering (HIPIMS and DCMS) together with synchronous biasing. HIPIMS serves here as a pulsed source of energetic heavy-metal-ions that are incident on the thin film deposited from DCMS sources to effectively eliminate porosity even if no external heating is used. G. Greczynski, J. Lu, I. Petrov, J.E. Greene, S. Bolz, W. Kölker, Ch. Schifflers, O. Lemmer and L. Hultman, J. Vac. Sci. Technol. A 32 (2014) 041515


A novel TiAlCN/CNx multilayer coating, consisting of nine TiAlCN/CNx periods with a top layer of CNx, was designed to enhance the corrosion resistance of CoCrMo biomedical alloy. B. Alemón, ..., E. Broitman, Nuclear Instruments and Methods in Physics Research B 331 (2014), 134–139

TECHNOLOGY TRANSFER AND INTERACTION

- Vinn Excellence Center FunMat
- ABB Corporate Research /Impact Coatings (spin-off by our graduate H. Ljungcrantz) for applications of contact materials; industry postdoc A. Flink
- SECO Tools, Sandvik Tooling, Ion Bond, SKF, CemeCon: research on wear-resistant films and PVD processes; industry PhD student L. Landälv
- DTI/Topsøe Fuel Cell A/S; industry PhD student S. Sønderby; resulted in gadolinia-doped ceria barrier layers available as product from DTI
- Patent application together with CemeCon AG: Dense, hard coatings on substrates using HIPIMS; G. Greczynski

- Studsvik Nuclear AB; novel oxide characterization method for nuclear plant reactor materials implemented with our Triboiindenter II-95c; E. Broitman
- N-works AB – spin-off company by Birch/Hultman
- Eurostars T-to-Power: R&D and commercialization of thermoelectric devices with Danish Technological Institute and TEGnology A/S [Eklund]
- MyFab National Access Grant [Hsiao]
- ESS AB collaboration on neutron detectors; [PhD student M. Imam]
- Partner of Excillum AB for the VInNOVA project (“materialbaserad konkurrenskraft”) “Boron Nitride as protective layer in X-ray tube” [Henry]
- Popular science article “Atomerna in på livet” Kemivärlden Biotech 11 2014 [Persson]
General Information

The program “Theory and Modelling (T&M)” at the Department of Physics, Chemistry and Biology (IFM) includes Theoretical Physics, Theoretical Chemistry, Theoretical Biology, and Bioinformatics. Though the disciplines at T&M represent broad scientific fields they all rely on a common core of mathematical modelling, 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.

The field of theory and modelling is 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 as in geophysics and astrophysics.

Also, the need for research and education in the broad field of theory and modelling is evidently great. 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.

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 modelling), Uno Wennergren (theoretical biology), Björn Wallner (bioinformatics), and Patrick Norman (theoretical chemistry). Lejla Kronbäck acts as administrative assistant. Members of T&M carry out innovative research. In 2014 we published 84 papers in international journals with referee system. Our papers are well cited.

Members of Theory and Modelling division at “Theory and Modelling Day” December 17, 2014

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 Centre (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 “Multifilms”, “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”. In 2015 Knut and Alice Wallenbergs Foundation gave its support to the project “Strong Field Physics and New States of Matter” that is coordinated by us.

T&M represents a broad and interdisciplinary research program. To find out more about each other’s research, we organize annual group meetings, “Theory and Modelling Day”. In 2014 we met on December 17 (see photo). Bioinformatics Division hosted the meeting, and organized the Theory and Modelling Christmas conference. The aim of the conference was to get knowledge about the different types of research and research projects conducted at T&M. Representatives from each of our divisions, theoretical physics, theoretical biology, theoretical chemistry, and bioinformatics, presented their research to a broader audience. We heard talks about how to computationally design molecular machines and new materials, how to make sense out of high-throughput biology experiments, as well as how important manure management will be to solve tomorrow’s food problems.

http://www.ifm.liu.se/theomod/
Bioinformatics

**STAFF**

*Senior lecturer:* Björn Wallner  
*BILS expert:* Malin Larsson (Ph.D.)  
*Post docs:* Claudio Mirabello, Sankar Basu  
*PhD. student:* Robert Pilstä  
*Administrative assistant:* Lejla Kronbäck  
*MSc student:* Denny Petersson, Dan Lee Vazquez Garcia, Martin Hyvönen

During 2014 have recruited two postdocs, Claudio Mirabello in March working predicting protein-protein interactions using large-scale modelling and structural alignment, and Sankar Basu in October working with development of machine learning methods that recognize good protein-protein interfaces. We have also had three master students in the group working on several aspects of protein docking and structure refinement.

The recruitment of the new senior lecturer in Bioinformatics is now done and we are happy to welcome Mika Gustafsson to our division, starting January 1. Mika has been working with gene networks and modules to understand disease at the medical faculty before.

**RESEARCH**

**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 pro-tein domain to predict interaction surfaces and ex-actly which residues that interact (cf. Figure 1). 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 seqs). This ac-curacy is enough to fold proteins without any structural homolog.

![Figure 1](image1.png)

*Figure 1:* Predicted residue contacts in the interface of a two domain protein highlighted in sticks, correctly predicted (gold), incorrect (red); domain 1 in white and domain 2 in black.

**Structural Calculations and Predictions**

We use molecular modelling techniques to study molecular interactions and sequence variations in relation to structural changes. In a joint project with the Sunnerhagen group at IFM, we have used molecular dynamics to explain how a single amino acid change in a protein called MexR (cf Figure 2) in the bacterium *Pseudomonas aeruginosa* change the protein dynamics, and leads to infections resistant to antibiotics.

**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 the quality assessment category in CASP10, the biennial community-wide Olympic games of protein structure prediction methods. Together with Randy Read in Cambridge, we are integrating our tools in the Phaser program to improve molecular replacement, the main technique to solve the phase problem in protein structure determination by x-ray crystallography.

**Teaching**

During 2014, we have arranged the bioinformatics course TFTB45.

**SeRC**

IFM Bioinformatics is very active in the Swedish e-Science Research Centre (SeRC), where Björn Wallner coordinates the bioinformatics community and represents Linköping University in the SeRC management group.

**BILS**

Bioinformatics Infrastructure for Life Sciences – is a national research infrastructure that provides bio-informatics support. Here at IFM Malin Larsson is the BILS expert, her main expertise is genetic variation, but support is also given in related areas. Last year support was given to groups in biostatistics, analysis of gene expression, genetic variation and massively parallel DNA sequence data.
Theoretical Biology

**STAFF**

**Professors:** Uno Wennergren (Head of division), Bo Ebenman  
**Associate professors:** Annie Jonsson, Anna Eklöf  
**Postdoc:** Tom Lindström, Amrei Binzer  
**PhD students:** Peter Brommesson, Alva Curtsdotter, David Gilljam, Sara Gudmundson, Stefan Sellman, Torbjörn Säterberg, Jonatan Årevall, Anna Åkesson  
**Administrative assistant:** Anna Sundin

**GENERAL INFORMATION**

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.

**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. 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 Algers (SLU), Prof Colleen Webb (Colorado State University), Dr Michael Tildesley (Warwick University) and Docent Susanna Sternberg Lwerin (SLU).

**EXTERNAL FUNDING**

Financial support has been received from the Swedish Research Council (VR), Swedish Research Council for Environment, Agricultural Sciences and Spatial Planning (FORMAS), VINNOVA, Swedish Agricultural Board, Swedish Emergency Management Agency, and Department of Homeland Security US.

**HIGHLIGHTS**

The SPABIO lab takes the final step to launch their logistic and route planning tool of animal transports. The project is done in collaboration with HKScan and Skogforsk. It is funded by Vinnova and the aim is to increase animal welfare and reduce costs and emission.

Anna Eklöf form a new group by hiring a postdoc, Amrei Binzer, and a PhD student, Anna Åkesson. The group focuses on the dynamics, robustness and functionality of large empirical and theoretical food webs. The group is funded by grants from VR and LiU.

[http://cms.ifm.liu.se/theomod/theobio.html](http://cms.ifm.liu.se/theomod/theobio.html)
Theoretical Chemistry

STAFF

Professors: Patrick Norman (Head of division), Sven Stafström
Associate professors: Magnus Boman, Gueorgui Gueorguiev, Bo Durbeej, Mathieu Linares, Joanna Kauczor
Postdocs: Jonas Björk, Chang-Feng Fang, Jaime Rosal, Florent Di Meo
PhD students: Jonas Sjöqvist, Cecilia Goyenola, Olle Falklöf, Thomas Fransson, Paulo Medeiros, Baswanth Oruganti, Riccardo Volpi, Morten Pedersen, Tobias Fahleson, Luiz Ribeiro, Renato Dos Santos, Rafael Freitas
Administrative assistant: Lejla Kronbäck

GENERAL INFORMATION

In our work to describe molecular structure and dynamics and electronic structure and motions in molecular materials, we employ 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 excited states and spectroscopic applications, the nudged elastic band (NEB) method for determining minimum energy paths and transition states, QM/MM methods for complex systems and environments, 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 carbon based but e.g. silicon based systems and III-nitrides are also modeled. Through our engagement in the broad Scandinavian collaboration centered around the Dalton software package (http://www.daltonprogram.org/) we take an active part in the development of new quantum chemical methods. Our research cuts across a range of disciplines (molecular and supramolecular electronics, photonics, materials and polymer science, surface 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.

We give a number of courses on undergraduate and graduate levels: Classical Mechanics (undergraduate, BD, MB), Quantum Mechanics (undergraduate, MB), Computational Quantum Chemistry (graduate, ML, BD), Molecular Mechanics and Molecular Dynamics (graduate, ML).

HIGHLIGHTS

- Toward a molecular understanding of the detection of amyloid proteins with flexible conjugated oligothiophenes in J. Phys. Chem. A 2014, 118, 9820
- Computational study of the working mechanism and rate acceleration of overcrowded alkene-based light-driven rotary molecular motors in RSC Adv. 2014, 4, 10240

COLLABORATIONS WITHIN LIU

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

EXTERNAL ACTIVITIES AND NETWORKS

- Secretary General, VR (SS)
- Board member, Nordforsk (SS)
- Director, NSC (PN)
- Steering group SeRC (PN)
- Faculty member, SeRC (ML)
- Co-authors, DALTON program (JK and PN)

INDIVIDUAL EXTERNAL COLLABORATIONS

- H. Ågren (KTH, Stockholm)
- T. Saue (Toulouse, France)
- F. Hanke (Accelrys, Cambridge, UK)
- K. Ruud (Tromsø, Norway)
- N. Avarvari (Angers, France)
- D. Beljonne (Mons, Belgium)
- R. Rivelino, F. Brito, C.M.C. de Castilho (Federal University of Bahia, Salvador, Brazil)
- Fernando Nogueira (Coimbra, Portugal)
- Zsolt Czigány (Budapest, Hungary)
- Micael Oliveira, (Liege, Belgium)
- J. Helliwell (Manchester, UK)
- J. Barth (Technische Universität München, Germany)
- M. Stöhr (Zernike Institute, Groningen, The Netherlands)
Theoretical Physics

STAFF

Professors: Igor Abrikosov (Head T&M), Karl-Fredrik Berggren, Magnus Johansson, Bo Sernelius, Sergei Simak, Irina Yakimenko
Associate Professor: Peter Münger
Assistant professors: Rickard Armiento, Weine Olovsson, Leonid Pourovskii, Ferenc Tasnádi, Marcus Ekholm
Postdoctoral fellows: Maxim Belov, Qingguo Feng, Olle Hellman, Peter Steneteg, Olga Vekilova, Zamaan Raza, Kati Finzel, Nuala Mai Caffrey
PhD student: Viktor Ivady, Peter Jason, Hans Lind, Alexander Lindmaa, Igor Mosyagin, Elham Mozfari, Fei Wang, Alexey Tal
Administrative assistants: Lejla Kronbäck
Masters students: Lasse Hultberg, Felix Faber
Bachelor student: Erik Johansson
Project student: Henrik Karlsson, Johan Klarbring
Visiting researchers: Prof. Lennart Stenflo, Dr. Alena Ponomareva (NUST “MISIS”, Moscow, Russia), Prof. Marc Cahay, Cincinnati University (USA), Andrey Lugovskoy (NUST “MISIS”, Moscow, Russia)

Appointments in 2014
- Ferenc Tasnádi has been appointed as Docent in theoretical and computational physics (from April, 27).
- Marcus Ekholm has been appointed as Lecturer (junior universitetslektor) (from July, 1)

GENERAL INFORMATION

The research in theoretical physics is focused on condensed matter physics/theoretical materials science, nanoscience, electromagnetic modelling, 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 (M. Ekholm, L. Pourovskii, Q. Feng, E. Mozfari, I. Abrikosov)
- Theoretical spectroscopy (W. Olovsson)
- Methodological development for computational density functional theory (R. Armiento, K. Finzel, A. Lindmaa, V. Ivady, I. Abrikosov)
- Materials modelling and high throughput energy material design (R. Armiento, A. Lindmaa, K. Finzel, I. Abrikosov)

EXTERNAL FUNDING

External funding is essential for the group activities. We are grateful for support from a number of sources including the Swedish Research Council (VR), European Commission, Foundation for Strategic Research (SSF), Knut and Alice Wallenberg Foundation (KAW), Carl Trygger Foundation, Wenner-Gren Foundations, Olle Engkvist Foundation and International Science Programme (ISP). In particular, Patrick Norman is coordinator for KAW project “Strong Field Physics and New States of Matter”, Bo Durbeej has a VR grant for young researchers, Mathieu Linares is a faculty member of 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. Our work has been enabled by the provision of high-performance computing resources by Swedish National Infrastructure for Computing (SNIC) and National Supercomputer Centre, NSC, at Linköping University.
• 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)
• Dynamics of nonlinear lattice models: Fundamental concepts and applications for optics, cold atoms and condensed matter (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)
• Gravitation as a Casimir interaction (B. E. Sernelius)
• Casimir effects in graphene systems (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 “Multifilms” and “FUNCASE”, both supported by the Swedish Foundation for Advanced Functional Materials, supported, by the Swedish Research Council. Also, we participate in projects “Isotopic Control for Ultimate Material Properties”, “Nanoparticles by Pulsed Plasma” and “Strong Field Physics and New States of Matter” supported by Knut and Alice Wallenbergs Foundation. At the European level, we were actively involved in European Network Psi-k, where Prof. Abrikosov is a Board of Trustees Member and a Spokesperson for Working Group “Real Materials: Metallic Alloys”.

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 classical mechanics, computational physics in physics education, electromagnetism, analytical mechanics, quantum theory, relativistic quantum mechanics, condensed matter physics, many-body physics, statistical mechanics, quantum information and computing, elementary particle physics, cosmology, quantum field theory, chaos and nonlinear phenomena. Peter Münger and Magnus Johansson take part in the EU Academic Network: Horizons of Physics Education (HOPE). It is a collaboration between more than 70 European University Physics Departments with the aim to investigate and improve various aspects of physics education. Karl-Fredrik Berggren and Irina Yakimenko are supervisors of a project for Felix Tellander and Johan Ulander, students at Berzelius gymnasium. They have won the competition “Unga forskare” at LiU, participated in Swedish competition in Stockholm and in the European competition in Warsaw (Poland).

**Licentiate Examination**

Peter Jason, “Comparisons between classical and quantum mechanical nonlinear lattice models”, Thesis No. 1648.

**AWARDS**

Gyllene Moroten LinTek Pedagogy Award to Peter Münger.

**HIGHLIGHTS 2014**


Controllable paramagnetic point defects in semiconductors exhibit enormous potential for nanometerology applications. In our highlighted publication, the promising features of a new candidate, the divacancy in SiC, have been explored by joint experimental and theoretical investigation. We utilized large-scale first principles calculation to study microscopic effects on the localized defect states as well as on the fine structure of the electron spin states due to the external electric field and strain. Our results provided useful insight to the physics of the defect, revealed the major role of the structural relaxation on the spin-spin interaction due to the applied strain, and the strengthening effect of the bulk polarization of the host semiconductor on the defect’s sensitivity for the variation of the external electric field.

**Figure 1:** Electric field effects on neutral-divacancy electron orbitals. The change of the ground state spin density of the divacancy in SiC (hh site) due to an external electric field of 0.1V/Å along the c-axis, with the electric field pointing upwards. The spin density is built from the charge densities of the double degenerate e orbitals localized on the C dangling bonds in the Si-vacancy part of the defect. Due to the external electric field, charge transfer occurs toward the dangling bonds of the C-atoms in the Si-vacancy part of divacancy from the dangling bonds of the Si-atoms in the C-vacancy part of divacancy.

**Phonon thermal transport in Bi₃Te₅ from first principles**
[O. Hellman and D. A. Broido, Phys. Rev. B 90, 134309 (2014)]

First-principles calculations of the thermal and thermal transport properties of Bi₃Te₅ that combine an ab initio molecular dynamics (AIMD) approach to calculate interatomic force constants (IFCs) along with a full iterative solution of the Peierls-Boltzmann transport equation for phonons have been performed. The newly developed AIMD approach allows determination of harmonic and anharmonic interatomic forces at each temperature, which is particularly appropriate for highly anharmonic materials such as Bi₃Te₅. The calculated phonon dispersions, heat capacity, and thermal expansion coefficient are found to be in good agreement with measured data. The lattice thermal conductivity calculated using the AIMD approach nicely matches measured values, showing better...
agreement than that obtained using temperature-independent IFCs. A significant contribution to the lattice thermal conductivity from optic phonon modes has been found. Already at room temperature, the phonon line shapes (see Figure) show a notable broadening and onset of satellite peaks reflecting the underlying strong anharmonicity.

Wave transport and statistical properties of an open non-Hermitian quantum dot with parity-time symmetry


A basic quantum-mechanical model for wave functions and current flow in open quantum dots or billiards is investigated. The model involves non-Hermitian quantum mechanics, parity-time (PT) symmetry, and PT-symmetry breaking. Attached leads are represented by positive and negative imaginary potentials. Thus probability densities, currents flows, etc., for open quantum dots or billiards may be simulated in this way by solving the Schrödinger equation with a complex potential. Here we consider a nominally open ballistic quantum dot emulated by a planar microwave cavity. The model is of conceptual as well as of practical and educational interest.


We derive a general procedure for finding the electromagnetic normal modes in layered structures. These normal modes are important in a variety of applications. They are the only input needed in calculations of Casimir interactions. We present an explicit expression for the condition for modes and Casimir energy for a large number of specific geometries. The layers are allowed to be two-dimensional as well as of two-dimensional electron gases can be handled within the formalism. Also, forces on atoms in layered structures are obtained. One side result is the van der Waals and Casimir-Polder interaction between two atoms.
• Karl-Fredrik Berggren, Joint Meeting of Advisory and Opportunities Committees, ERC Programme Grant – Nanoelectronic Based Quantum Physics-Technology and Applications, University College London (UCL), UK.

**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. Neugebauer (Max-Planck-Institut für Eisenforschung, Germany).

• Igor Abrikosov, Viktor Ivady, Rickard Armiento and Dr. Adam Gali (Hungarian Academy of Sciences).

• Bo Sernelius with Prof. G. D. Mahan (Penn State University, USA), Prof. Antonio Ferreira da Silva (Salvador de Bahia, Brazil), Prof. Barry Ninh (Australian National University, Australia), Prof. Chris Binns (University of Leicester, England), Dr. Mike Ward, University of Birmingham, Birmingham, UK, Dr. Astrid Lambrecht, École Normale Supérieure, Paris, France, Prof. Clas Persson and Dr. Mathias Boström (University of Oslo, Norway), and Prof. Iver Brevik (Norwegian University of Science and Technology, Norway).

• Magnus Johansson with Dr. S. Dereyanko (Weizmann Institute of Science, Israel), Dr. Y. Prylepskyi (Aston University, UK), the group of Dr. R.A. Vicencio and Prof. M.I. Molina (Universidad de Chile, Santiago), and the group of Prof. M. Stepic and Prof. A. Maluckov (Vinca Institute, Belgrade, Serbia).

• Sergei Simak and Prof. O.M. Krasilnikov, Prof. Yu.Kh. Vekilov at NUST “MISIS”, Russia, Prof. N.V. Skorodumova at KTH.

• Leonid Pourovskii 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, with Prof. J. Bird (University of Buffalo, USA) and Prof. M. Cahay (Cincinnati University, USA).

• Peter Münger, collaboration with Anna Eklöf, University of Basel, Switzerland).

• 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 Armiento and Ann E. Mattsson (Sandia National Laboratories, USA), Gerbrand Ceder (Massachusetts Institute of Technology, USA), Stephan Kümmel (University of Bayreuth, Germany), Predag Lazić (Rudjer Boskovic Institute, Croatia), Marco Fornari (Central Michigan University, USA), Boris Kozinsky (Robert Bosch LLC, USA), Anatole von Lilienfeld (Argonne National Laboratories, USA), Boris Kozinsky (Robert Bosch LLC, USA), Anatole von Lilienfeld (Argonne National Laboratories, USA) and École Polytechnique, Paris, France.

• Maxim Belov spent one month at the École Polytechnique in Paris, France.

• Olle Hellman visited Oak Ridge National Laboratories, USA, to initiate collaboration on thermal conductivity simulations.

• Viktor Ivady had a long-term visit to Hungarian Academy of Sciences.

• Igor Abrikosov visited NUST “MISIS”, Moscow and Tomsk State University, Russia.

• Leonid Pourovskii has shared employment between IFM and École Polytechnique, Paris, France.

• Sergei Simak visited NUST “MISIS”, Russia.

• Weine Olovsson made a visit to Japan for discussions about collaboration at Kyoto University, University of Tokyo and Spring8. Other visits were to the Humboldt Universität zu Berlin.

• Karl-Fredrik Berggren, Seminar at Fakultät für Physik, Ludwig-Maximilians-Universität, München.

**International conferences**

• Igor Abrikosov gave invited talks at Asia Sweden meeting on understanding functional materials from lattice dynamics (ASMFLD 2014), Guwahati, India; The 27th Conference of the Israel Nuclear Societies, Ein Bokek, Israel; 13-th International Ceramics Congress CIMTEC2014, Montecatini Terme, Italy; CMD25 - JCM14, Paris, France; 52nd European High Pressure Research Group International Meeting Lyon, France.

• Igor Abrikosov gave keynote talks at International Conference “Science of the future”, St. Petersburg, Russia and at International workshop on Ab initio Description of Iron and Steel (ADIS2014): Multiple impacts of magnetism, Ringberg Castle, Germany.

• Weine Olovsson gave an invited talk at “How Exciting 2014”, Berlin, Germany.


• Magnus Johansson was Invited speaker at the EPSRC Workshop on Non-Equilibrium Processes at Negative Temperature, Glasgow 23-24 October.

**POPULARIZATION OF SCIENCE**

• Start page of our group web-site http://www.ifm.liu.se/theomod/theophys/ is used to present highlights of our recent research for the general public.

• Karl-Fredrik Berggren, interview “CERN 60 years” Sveriges Radio, Studio Ett, 2014-09-10


• Marcus Ekholm was consulted by Skolinspektionen.

https://www.ifm.liu.se/theomod/theophys/
RESEARCH CENTRES
AFM

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

Director: Prof. Magnus Berggren (ITN) (Prof. Lars Hultman leave of absence June 2013)
Deputy director: Prof. Igor Abrikosov
AFM encompasses 250 researchers from the departments IFM, ITN and IEI, and a partner ACREO, organized into interactive collaborating teams.

MANAGEMENT BOARD:
- Magnus Berggren (Chair)
- Igor Abrikosov (Vice Chair)
- Jens Birch
- Erik Janzén
- Kajsa Uvdal
- Per Olof Holtz
- 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 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)


HIGHLIGHTS 2014
- A 300 delegate AFM conference with invited international speakers, opened by LiU Vice Chancellor, was held in Kolmården 20 to 21 of August.
- The Graduate School Agora Materiae in Materials Science has grown to a record high enrollment of 47 PhD students.
- 268 peer-reviewed publications (213 in 2013), including three Nature Materials:
  1. Semi-metallic polymers
  2. Isolated electron spins in silicon carbide with millisecond coherence times
  3. Coherent control of single spins in silicon carbide at room temperature
- We designed and constructed a new sublimation growth reactor for fabrication of large-area graphene on SiC. Substrate diameters up to 100 mm can be used. Its inauguration is expected in April 2015. This reactor is exploited in collaboration with our spin-off company Graphenics AB.
- Our research on graphene made breakthroughs: (i) discovery that graphene grown on cubic SiC – substrates are produced in our lab – is less doped from the substrate as compared with hexagonal substrates due to the absence of
CeNano

The Centre in Nano Science and Technology (CeNano) is an organisation within Linköping Institute of Technology (LITH) at Linköping University. The mission of CeNano is to strengthen and support the competence within nano science and nano technology of the faculty. This is done by gathering researchers with nano activities in the centre and by acting for increased collaborations and joint 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.

In November 2014, the 10th CeNano Symposium was organized, a full day of 17 project presentations by PhD students benefiting from CeNano support. Invited speaker was Dr Jakub Dostalek, Austrian Institute of Technology GmbH, Vienna.

THE BOARD OF CENANO:

- Kajsa Uvdal, Chair
- Daniel Aili
- Jens Birch
- Per Hammarström
- Per-Olof Holtz
- Sergei Simak
- Karin Enander, Director

Projects granted support by CeNano 2014:

- Imaging strategies for dynamic and responsive supramolecular nanostructures by applying low-kV and in-situ transmission electron microscopy PIs: Daniel Aili and Per Persson
- The missing link between theory and experiment for the understanding of the nanostructure of amorphous boron carbide PIs: Björn Alling and Henrik Pedersen
- Biocompatibility studies of engineered nanoparticles aimed for use in biomedical applications PI: Caroline Bromnsson
- Tailoring the light emission efficiency of ZnO nanoparticles via polymer coating for optoelectronic applications PI: Volodymyr Khranovskyy
- Investigating magnetron sputter epitaxy of ZrB2 on MOCVD grown GaN epi-layers for potential use in High Electron Mobility Transistors PIs: Urban Forsberg and Hans Högberg
- Organic/inorganic hybrid structures fabricated utilizing III-N nanorods PI: Galia Pozina
- Designed nanoparticles for graphene-based gas sensors PI: Rickard Gunnarsson
- Boron nitride - the ultimate substrate for graphene PI: Anne Henry
- Synthesis and Characterization of chiral organic nanostructures PI: Kenneth Järrendahl
- Nanomechanical and nanodynamic properties of protein entities participating in dynamic conformational selection and multimodal recognition PI: Maria Sunnerhagen
• Ultrabright semiconducting polymer dots (Pdots) for specific cancer cell targeting PI: Xuanjun Zhang
• Sum decomposition of Mueller matrices of biological nanostructures PI: Hans Arwin
• Interface coherency studies in c-Ti1-xCrxN/h-AlN and c-Ti1-xZrxN/h-AlN (x=0-1) multilayers PIs: Naureen Ghafoor and Ferenc Tasnádi
• Eu-doped Gd2O3 nanoparticles for specific dual-modal biomedical imaging PI: Zhangjun Hu
• Developing a smart electronic paper based on piezoelectric nanowires PI: Omer Nour
• Surface diffusion studies of non-carbide forming adatoms on graphene surfaces PIs: Per Persson and Vanya Durakchieva
• Registration of nanoparticle-microelectrode collisions: electroanalysis for nanomaterials characterization and environmental monitoring PIs: Mikhail Vagin and Martin Mak

HIGHLIGHTS

Ultrabright semiconducting polymer dots (Pdots) for specific cancer cell targeting

Peter Eriksson and Xuanjun Zhang

Semiconducting polymer nanoparticles (Pdots) are a new class of fluorescent nanoprobe with superior characteristics such as low toxicity, ultra bright photoluminescence, non-blinking, and fast emission rates. We are now developing reliable methods to (1) functionalize the Pdot surface for specific bioconjugation with biomolecules such as proteins, cancer drugs, antibodies, etc; (2) tune emission to Near-Infrared (NIR) region for practical in vivo applications. The bright NIR fluorescent Pdots with specific targeting ligands are very promising for a variety of biological applications.

Mathias Forsberg and Galia Pozina

Hybrid structures based on III-N semiconductor quantum well (QW) and organic polymers utilizing non-radiative resonant energy transfer (NRET) from excitations generated in QW to excitons in the fluorescent layer have potential applications as efficient emitters for down converting of UV and blue light. In this project a new design of hybrid will be used: organic polyfluorenes with emission in visible region deposited on heterostructured AlInN/GaN nanorods produced by DC magnetron sputtering.

Organic/inorganic hybrid structures fabricated utilizing III-N nanorods
FunMat

VINNOVA Excellence Center in Research and Innovation on Functional Nanoscale Materials

FunMat is in equal parts financed by VINNOVA, industry and the university. The Center runs between 2007 and 2016 with the mission to:

- Provide the strongest research platform for a consortium of companies in the area of advanced surface engineering, with a focus on nanotechnology for tools, components, contacts, and sensors
- Offer knowledge-based design of functional materials on the nanoscale to provide unique and improved surface properties with commensurate industrial opportunities
- Expand core R&D capabilities by enlarging and protecting the IPR base of Sweden-operating companies in key industrial sectors.

The Center is based at IFM, Linköping University.

RESEARCH PROGRAM

FunMat is a leading environment for problem-oriented research on nanoscale functional materials. It offers scientific competence and innovative solutions in advanced surface engineering. We develop thin film processing, advanced materials analysis, sensors and IPR.

PROJECT THEMES

- **Multifunctional Nanocomposites for Combined Electric and Mechanical Contacts.** We develop novel coating materials for electrical contact applications. The nanocomposite MaxPhase coating materials replace gold in electrical contacts. They are tough, electrically conducting, resistant to corrosion and wear, cheap, and environmentally friendly – truly multifunctional materials.

- **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 drive innovations in hybrid HiPIMS/DCMS processing for advanced surface engineering, including coating/substrate adhesion optimization. Target applications are transition metal nitrides and resilient fullerene-like C-based coatings. Expertise is provided on PVD deposition, plasma characterization, XPS, electron microscopy, nanotribology, as well as theoretical calculations.

NEW NANOSCALE SENSOR MATERIALS & APPLICATION

The conducting ceramic materials developed in FunMat offers a unique possibility for silicon carbide sensors and other challenging sensor de-velopments. Specifically, silicon carbide chemical sensors are commercialized for applications in harsh environment. In the FunMat center we de-velop ohmic contacts for temperatures ≥ 500°C and sensors e.g. for NH₃, SO₂, H₂S, NOₓ and soot. Epitaxially grown graphene on SiC, decorated with nanoparticles of metals and metal oxides, is developed as ultra-sensitive gas sensors for envi-ronmental applications.
Graphene/SiC decorated by metal particles for gas sensing

HIGHLIGHTS 2014

• Prof. Anita Lloyd Spetz was awarded the Junior Faculty Price 2014 at Linköping University.

• The generic knowledge gained in FunMat has been implemented in new manufacturing pro-cesses at partner companies. These processes are used in a large number of products. The gained knowledge is also used to drive their material suppliers to provide tailor-made cathode materials.

• Impact Coatings have commercialized the coating combinations Ceramic MaxPhase and Silver MaxPhase and also several deposition sys-tems.

• Amorphous carbide thin films crystallize during high-resolution TEM imaging. These results are profoundly im-portant for any investigation of amorphous coating materials, as great care must be taken to avoid inducing artifacts by electron microscopy.

• Decreasing grain size of cathodes improves properties of coatings.

• Novel nanolabyrinthine structure of ZrAlN results in extreme hardness.

• CemeCon AG, is finalizing the development of a new coating family based on the patented solu-tions, and knowledge generated in FunMat is used to design their next generation of deposition systems based on the HIPIMS technology.

• CNx coatings deposited at LiU on SKF test rollers show 40% reduction in the friction coef-ficient.

• Films with high hardness can be deposited on temperature-sensitive substrates (e.g. plastics).

• SiC based sensors have been commercialized and are de-veloped within the center for SO2, CO, O2, NOx, NH3 and PM sensors.

• An improved SiC-FET device detected formaldehyde, benzene, naphthalene at ppb levels.

• Ti3SiC2 is developed as ohmic contact to SiC. Deposition from only one target simplifies pro-cessing and facilitates mass production.

• SiC-FET in T-cycled operation mode + smart data evaluation enables SO2 monitoring in a de-sulphurisation system in a power plant.

• Graphene on SiC, with TiO2 nanoparticles, responded to ppb levels of formaldehyde and benzene, particle size provide selectivity.

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. Anita Lloyd Spetz (Head, Theme 5 Leader)
Prof. Magnus Odén (Deputy Head, Theme 2 Leader)
Assoc. Prof. Per Eklund (Research Coordinator, Theme 1 Leader)
Assoc. Prof. Grzegorz Greczynski (Theme 4 leader)
Ms. Therese Dannetun (Coordinator)
Prof. Emerita Rosiţa Yakimova (Senior Advisor)
Prof. Lars Hultman (Senior Advisor, Founder of FunMat, Head until June 2013, now Director of SSF)

Partner Companies

Senior Researchers: Mike Andersson, Robert Bjorklund, Esteban Broitman, Vanya Darakchieva, Jens Eriksson, Naureen Ghafoor, Gueorgui Gueorguiev, Hans Hägberg, Ulf Jansson (at Uppsala University), Anelia Kakanakova, Jun Lu, Per Persson, Galia Pozina, Donatella Puglisi

Research Engineers: Thomas Lingefelt, Peter Moller

PhD students: Konstantinos Bakoglidis, Zhaferia Darmastuti (PhD June 2014), Hossein Fashandi, David Engberg, Nils Nedfors (at Uppsala Univ, PhD April 2014), Bilal Syed, Olof Tengstrand (PhD March 2014), Jennifer Ullbrand

Post-docs: Axel Flink (until February 2014), Lina Rogström, Jianqiang Zhu, Zhaferia Darmastuti (from July 2014)

University collaborations: Uppsala University, University of Illinois (USA)

www.liu.se/forskning/funmat
Linköping Linnaeus Initiative for Novel Functional Materials (LiLi-NFM)

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**
Pro. Erik Janzén (acting)
Pro. Lars Hultman (leave of absence)

**Deputy Director**
Pro. Mats Fahlman

**Scientific Secretary**
Pro. Irina Yakimenko

**Coordinator:** Ms. Malin Wahlberg

**Research Divisions and Principal Investigators**

**Theoretical Chemistry:** Prof. Sven Stafström  
**Functional Electronic Materials:** Prof. Weimin Chen, Prof. Irina Buyanova

**Nanostructured Materials:** Prof. Magnus Odén  
**Plasma & Coating Physics:** 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. Roger Uhrberg, Prof. Wei-Xin Ni, Prof. Göran Hansson

**Surface Physics and Chemistry:** Prof. Mats Fahlman,  
**Theory and Modeling:** 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 which is funded by EC. 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

**STRATEGIC RECRUITMENTS**

Olle Kordina, Per Eklund, Jens Jensen, Mathieu Linares, Daniel Dagnelund, Martin Magnuson, Weine Olövsson, Henrik Pedersen, Iris Pilch, Fredrik Söderlind, Daniel Söderström, Jan Stehr, Rickard Armiento, Volodymyr Khranovskyy, Yuttapoom Puttisong.
LILI-NFM WORKSHOPS

• *on Advanced Materials Analysis* organized by Advanced Materials Analysis Platform Lili-NFM, Linköping University, 3-4 June 2014 (organizers: Prof. J. Birch, Prof. R. Uhrberg and Prof. I. Yakimenko), 35 participants.

LILI-NFM SEMINARS SERIES

In 2014 presentations were given by Dr. Per Persson, Thin Film Physics, IFM, Dr. Yuttapoom Puttisong, Functional Electronic Materials, IFM, Prof. Clivia M. Sotomayor Torres, ICREA and Catalan Institute of Nanotechnology, Barcelona, Spain; KTH, School of ICT, Department of Materials and Nanophysics, Kista, Sweden, Prof. Marc Cahay, Spintronics and Vacuum Nanoelectronics Laboratory, University of Cincinnati, Cincinnati, USA, Prof. Stephen E. Saddow, Electrical Engineering Department University of South Florida, Tampa, USA, Dr. Xianjie Liu, Surface Physics and Chemistry, IFM.

SCIENTIFIC HIGHLIGHTS


We identify hyperfine-induced electron and nuclear spin cross relaxation as the dominant physical mechanism for the longitudinal electron spin relaxation time \( T_1 \) of the spinfiltering \( Ga\text{\textsuperscript{2+}} \) defects in GaNAs alloys. This conclusion is based on our experimental findings that is insensitive to temperature over 4-300 K and its exact value is directly correlated with the hyperfine coupling strength of the defects that varies between different configurations of the \( Ga\text{\textsuperscript{2+}} \) defects present in the alloys. These results thus provide a guideline for further improvements of the spin-filtering efficiency by optimizing growth and processing conditions to preferably incorporate the \( Ga\text{\textsuperscript{2+}} \) defects with a weak hyperfine interaction and by searching for new spin-filtering defects with zero nuclear spin.

![Image](339x301 to 518x457)

Figure 1: (a) and (b) Hanle curves (the open circles) obtained at RT from two GaNAs samples. The solid lines are the simulation curves obtained by a best fit of the coupled rate equations to the experimental data, with the specified fitting parameters of \( T_1^{\text{eff}}, T_\perp^{\text{eff}} \) estimated from the effective Hanle width. (c) and (d) Optically detected magnetic resonance (ODMR) spectra of the \( Ga\text{\textsuperscript{2+}} \) defects obtained at 4 K from the same samples as shown in (a) and (b). The solid lines are the simulation curves obtained by a best fit of the spin Hamiltonian to the experimental data. (continued)

Figure 1 (continued): The involved configurations of the \( Ga\text{\textsuperscript{2+}} \) defects are given in (c) and (d), together with the degrees of their contributions and the resulting average hyperfine parameter \( \langle A_\text{eff} \rangle \). The microwave frequencies used in ODMR are 33.92 GHz in (c) and 9.27 GHz in (d). [e] \( \langle A_\text{eff} \rangle \) as a function of \( 1/T_1^{\text{eff}} \), with each symbol representing a specific sample. The solid line is a linear fitting following the Fermi-golden rule. The dotted lines mark the associated parameters of each \( Ga\text{\textsuperscript{2+}} \) configuration, obtained from the rate equation and spin Hamiltonian analysis of the experimental data.


We show that defects formed in bulk and nanostructured ZnO synthesized using standard growth techniques promote efficient energy upconversion via two-step two-photon absorption (TS-TPA). From photoluminescence excitation (PLE) of the anti-Stokes emissions, the threshold energy of the TS-TPA process is determined as being 2.10 - 2.14 eV in all studied ZnO materials irrespective of the employed growth techniques. Our photo-electron paramagnetic resonance (EPR) studies show that this threshold closely matches the ionization energy of the zinc vacancy – a common grown-in intrinsic defect in ZnO, thereby identifying the zinc vacancy as being the dominant defect responsible for the observed efficient energy upconversion. The upconversion is found to persist even at a low excitation density, making it attractive for photonic and photovoltaic applications.

![Image](43x134 to 278x321)

Figure 2: PLE spectra measured at 5 K by monitoring the dominant upconverted emission from the bulk (a) and NWs (b) samples. The inset in (b) is a schematic picture of the TPA and TS-TPA processes via virtual and real defect (zinc vacancy) states, which are labeled as VS and \( (V_{Zn}) \), respectively. (c) Intensities of the detected EPR signals as a function of excitation wavelength.


The elimination of defects from silicon carbide (SiC) has facilitated its move to the forefront of the optoelectronics and power-electronics industries. Nonetheless, because certain SiC defects have electronic states with sharp optical transitions, they are increasingly recognized as a platform for quantum information applications, such as secure communication and quantum computing where the states of an intrinsic angular momentum of electrons, often called spin, are used as quantum bits. Research teams at Linköping, Takasaki, and Chicago have successfully designed and fabricated 4H-SiC single crystal samples with the divacancy (missing neighboring Si and
C atoms, see Figure 3) at low concentrations so that single divacancies can be isolated and coherently controlled. Bound to neutral divacancy defects, these states exhibit exceptionally long ensemble spin coherence times, exceeding 1 ms. Coherent control of single spins in a material amenable to advanced growth and microfabrication techniques is an exciting route towards wafer-scale quantum technologies.

Figure 3: 4H-SiC crystal structure showing four non-equivalent forms of divacancies, which consist of neighboring Si and C vacancies at the hexagonal (h) and quasi-cubic (k) sites.


The chemical robustness, wide optical transparency, and high carrier mobilities make (boron-doped) nanocrystalline diamond film as a good choice of the conductive transparent electrode in dye sensitized photovoltaics. It is still a challenge to directly graft the dye molecule on the diamond surface. Here we demonstrated that N3 dye molecules [cis-bis(isothiocyanato)bis(2,2’-bipyridyl-4,4’-dicarboxylato)ruthenium(II)] are covalently attached to boron-doped nanocrystalline diamond (B:NCD) thin films through a combination of coupling chemistries, i.e., diazonium, Suzuki, and EDC–NHS. X-ray and ultraviolet photoelectron spectroscopy and near-edge X-ray absorption fine structure spectroscopy are used to verify the covalent bonding of the dye on the B:NCD surface (compared to a hydrogen-terminated reference). The spectroscopic results confirm the presence of a dense N3 chromophore layer, and the positions of the frontier orbitals of the dye relative to the band edge of the B:NCD thin film are inferred as well. Proof-of-concept photoelectrochemical measurements show a strong increase in the photocurrent compared to non-dye-function alized B:NCD films. This study opens up the possibility of applying N3-sensitized B:NCD thin films as hole conductors in dye-sensitized solar cells.

Bonding, charge rearrangement and interface dipoles of benzene, graphene, and PAH molecules on Au(111) and Cu(111) [Paulo V. C. Medeiros, G. K. Gueorguiev, S. Stafström, CAR-BON 81, 520 (2015)]

We perform a theoretical study of the electronic properties of polyaromatic hydrocarbon (PAH) molecules, as well as benzene and graphene, adsorbed on copper and gold. The PAH molecules studied are coronene (C24H12), circumcoronene (C54H18) and circumcircumcoronene (C96H24), which we consider as gradual approximations to an infinite graphene layer. In order to understand how the size of the adsorbed PAH molecules influences the adsorbate-metal interactions, we generalize the approach used in our earlier study [Phys Rev B, 85 (2012), p. 205423] to decompose the binding energies and net charge transfers into separate contributions from specific groups of atoms, and we then show that the zigzag edges of the PAH molecules interact stronger with the metal surfaces than the armchair ones. We discuss the nature of binding in our model systems as well as the formation of interface dipoles. We show that for all model systems studied here, the charge rearrangement contribution to the interface dipoles can be expressed as the product of the charge involved in the formation of the dipole and the distance between well-defined centers of charge for electron accumulation and depletion. This distance is only marginally dependent on the specific PAH molecules, decreasing slowly with their size.

Figure 4: Left panel: The sketch of N3 dye molecule on Boron-doped diamond surface. Right panel: Comparison of NEXAFS spectrum of N3 dye functionalized B:NCD film with those of pure B:NCD film and pure N3 dye molecule. Dashed lines indicated the influence of the empty π* orbitals upon functionalization while the empty σ* orbitals were kept unchanged.

Figure 5: Equilibrium geometries of C54H18 and graphene adsorbed on Au(111) (upper panels) and Cu(111) (lower panels).

Acceptor doping of zinc oxide (ZnO) is the main challenge for the further application of the material in light emitting devices (LEDs). ZnO nanorods with excess of Ag as a possible acceptor dopant were fabricated by MOCVD growth at Linköping University by Dr. V. Khranovskyy. Influence of Ag on the structural and optical properties of nanorods was studied by high resolution transmission electron microscopy (HRTEM) and photoluminescence spectroscopy (PL). Ag incorporation into ZnO up to 0.4 at.% promote appearance of basal plane stacking fault (BSF) defects every ~12 nm and promotes corrugation of the side facets of the NRs. Presence of BSFs defects result in the specific photoluminescence peak (~386 nm), in addition to commonly observed near band edge (NBE) emission of ZnO (~375 nm). The BSFs defects concentration correlates strongly with the intensity of the additional emission peak, suggesting on their common origin. This finding contributes to the defect engineering in wide band gap semiconductors as well as promotes the further progress of ZnO as the alternative material for future LEDs.


Boron carbide is a class of materials, which is important for several applications. In particular, the high cross section for thermal neutron reaction of the isotope ¹⁰B makes boron carbide relevant as a new generation of neutron detectors, possibly replacing the present dominating He-based technologies suffering from the “He crisis”. We have studied the configurationally disordered crystalline boron carbide, with the composition B₄C from first-principles calculation, in both dilute and high concentration limit of carbon-boron substitutional defects. For the latter purpose, we have suggested a superatom’s picture (see Figure 7) of the complex structure and combined it with a special quasirandom structure approach for disorder. In this way, we have identified low-energy defects: (1) bipolar defects and (2) rotation of icosahedral carbon among the three polar-up sites. Further, two configurational phase transitions from the ordered to the disordered configurations have been predicted to take place upon an increase in temperature. The first transition, at 870 K, induces substitutional disorder of the icosahedral carbon atoms among the three polar-up sites; meanwhile the second transition, at 2325 K, reveals the random substitution of the icosahedral carbon atoms at all six polar sites coexisting with bipolar defects. The restoration of inversion symmetry after the second transition, yielding the full rhombohedral symmetry on average, agrees well with the experimental data reported in the literature. The electronic structure, calculated for the disordered phases, indicates a sensitivity of the band gap to the degree of configurational disorder in B₄C.

Figure 6: SEM image of Ag-doped ZnO nanorod with corrugated side facets (left upper image). The observed corrugation is accompanied by a high concentration of basal plane stacking faults (right upper image with the scale bar 5 nm). Micro-photoluminescence spectra from different positions of the ZnO:Ag NRs sample (bottom image). The mapped area is shown in the inset, where the excited points are marked. Spectrum assigned as position 1 is obtained by excitation of the top planes of ZnO NRs, while positions 2–6 correspond to excitation of areas of both top and side planes of NRs. Position 7 corresponds to excitation of only the side facets of a NR.


We grew epitaxial B₄ NaCl-structure V₁₋ₓWₓN /MgO(001) thin films with 0 ≤ x ≤ 0.60. The Gibbs free energy of mixing, calculated using DFT, reveals that cubic V₁₋ₓWₓN solid solutions with 0 ≤ x ≤ 0.7 are stable against spinodal decomposition and separation into the equilibrium cubic-VN and hexagonal-WN phases. We showed experimentally that alloying VN with WN leads to a monotonic increase in relaxed lattice parameters, enhanced nanoinindentation hardnesses, and reduced elastic moduli. Calculated lattice parameters and elastic moduli (obtained from calculated C₁₁, C₁₂, and C₄₄ elastic constants) are in agreement with experimental results. The observed increase in alloy hardness, with a corresponding decrease in the elastic modulus at higher x values, combined with DFT-calculated decreases in shear to bulk moduli ratios, and increased Cauchy pressures (C₁₁–C₄₄) with increasing x reveal a trend toward increased toughness.

We found that Ti adatoms on TiN(001) surfaces migrate between neighboring fourfold hollow sites primarily along in-plane <100> channels (see Figure 8). <100> and <110> single jumps, as well as <100> double jump rates, obtained directly from MD runs as a function of temperature, are used to determine diffusion activation energies $E_a$, and attempt frequencies $A$, for the 3 preferred Ti adatom migration pathways on TiN(001). From transition rates $A \exp[-E_a / (k_BT)]$, we determine adatom surface distribution probabilities as a function of time, which are used to calculate adatom diffusion coefficients $D_s(T)$. AIMD and CMD predictions are consistent and complementary. Using CMD, we investigate the effect on the adatom jump rate of varying the phonon wavelength degrees of freedom by increasing the supercell size. Long-wavelength phonons contribute to increasing adatom mobilities at temperatures up to 600 K. By directly tracking the Ti adatom mean-square displacement during CMD runs, we find that Ti adatom jumps are highly correlated on TiN(001), an effect that yields lower $D_s(T)$ values ($D_{corr}(T)=4.5 \times 10^{-4} \text{ cm}^2 \text{s}^{-1}$) $\exp[-0.55 \text{ eV} / (k_BT)]$.

Figure 8: Adsorption energy landscapes for Ti adatoms on a TiN(001) surface unit cell

Ti and N adatom Decent Pathways to the Terrace from atop 2D-TiN/TiN(001) Islands [D. Edström, D.G. Sangiovanni, L. Hultman, V. Chirita, I. Petrov, J.E. Greene, Thin Solid Films 558, 37 (2014)]

We use classical molecular dynamics and the modified embedded atom method to determine residence times and descent pathways of Ti and N adatoms on square, single-atom-high, TiN islands on TiN(001) (see Figure 9). Simulations are carried out at 1000 K, which is within the optimal range for TiN(001) epitaxial growth. Results show that the frequency of descent events, and overall adatom residence times, depend strongly on both the TiN(001) diffusion barrier for each species as well as the adatom island-edge location immediately prior to descent. Ti adatoms, with a low diffusion barrier, rapidly move toward the island periphery, via funneling, where they diffuse along upper island edges. The primary descent mechanism is via push-out/exchange with Ti island-edge atoms, a process in which the adatom replaces an island edge atom by moving down while pushing the edge atom out onto the terrace to occupy an epitaxial position along the island edge. Double push-out events are also observed for Ti adatoms descending at N corner positions. N adatoms, with a considerably higher diffusion barrier on TiN(001), require much longer times to reach island edges and, consequently, have significantly longer residence times. N adatoms are found to descend onto the terrace by direct hopping over island edges and corner atoms, as well as by concerted push-out/exchange with N atoms adjacent to Ti corners. For both adspecies, we observe several complex adatom/island interactions, before and after descent onto the terrace, including two instances of Ti island-atom ascent onto the island surface.

Figure 9: Net Ti adatom migration around a Ti-corner of a TiN/TiN(001) island via concerted motion of the adatom and corner atom along a [110] channel. Note that only part of the 8x8 atom island is shown. (a) Ti adatom has descended from the island via pushout/exchange next to the Ti corner, (b) the displaced Ti corner atom and descended Ti adatom both move in the [1 -1 0] direction, and (c) the displaced Ti corner atom returns to the corner position and the Ti adatom moves to the opposite epitaxial position adjacent to the Ti corner.


We screened a large chemical space of perovskite alloys for systems with optimal properties to accommodate a morphotropic phase boundary (MPB) in their composition-temperature phase diagram, a crucial feature for high piezoelectric performance. The screening started from alloy end points previously identified in a high-throughput computational search. An interpolation scheme was used to estimate the relative energies between different perovskite distortions for alloy compositions with a minimum of computational effort. Suggested alloys were further screened for thermodynamic stability. The screening identified alloy systems already known to host an MPB and suggests a few others that may be promising...
candidates for future experiments. Our method of investigation may be extended to other perovskite systems, e.g., (oxy-)nitrides, and provides a useful methodology for any application of high throughput screening of isovalent alloy systems.

Stability (upper graph) and energy preference for TET distortion (lower graph) in eV / atom for relevant alloys with Li with the components of the (K, Na)(Nb, Ta)O 3 system. The system becomes less stable the more Li is added, but it also more strongly prefers the TET distortion.

Crystallization Characteristics and Chemical Bonding Properties of Nickel Carbide Thin Film Nanocomposites


The amorphous structure, crystallization characteristics, chemical bonding, and electrical properties of magnetron sputtered nickel carbide Ni1-xCx nanocomposites have been investigated for a wide range of carbon contents. The crystallinity of the films was found to be strongly dependent on the carbon content and additional graphene-like structures are found at high carbon content. X-ray diffraction and X-ray absorption studies reveal carbon-containing hcp-Ni (hcp-NiCy phase), instead of the expected rhombohedral-Ni3C phase. The X-ray absorption spectra exhibit an increasing number of unoccupied Ni 3d states and a decreasing number of C 2p states as a function of carbon content. The spectral changes in X-ray absorption signify a systematic redistribution in orbital occupation due to charge-transfer effects at the domain-size-dependent carbide/matrix interfaces. These findings open new possibilities for modifying the resistivity of amorphous thin film coatings based on transition metal carbides through the control of amorphous domain structures. It is also shown that the resistivity is not only governed by the amount of carbon, but increases by more than a factor of two when the samples transform from crystalline to amorphous.

Figure 11: X-ray diffractograms of Ni1-xCx films with C content ranging from 4.9 to 61.8 at%. With increase of carbon content from 4.9 to 16.3 at%, the fcc-NiCx structure disappears and single phase hcp-NiCy forms, while for higher carbon contents the films are amorphous.


The influence of the surrounding cavity on the efficiency of different types of polaritonic emitters of THz radiation has been analysed. It is demonstrated that THz lasing threshold in realistic structures cannot be achieved without a THz cavity, due to destruction of polaritons via excitonic Mott transition. Two theoretical models have been considered: (i) when spontaneous emission rate of polaritons is proportional to the cavity Q-factor, and (ii) when the rate of emission is fixed. Embedding polaritonic microcavity into a cavity for the THz radiation provide a THz lasing even with a moderate Q-factor (up to 50) at pumping levels corresponding to the polariton densities below the excitonic Mott transition.

Figure 12: Schematic drawing of the structure for a polaritonic THz emitter: polaritonic microcavity with a quantum well is placed into the THz cavity.
STAFF

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GENERAL INFORMATION

The Linköping Biosensors and Bioelectronics Centre was established in 2010, with the objective of bringing together the many competences, activities and resources at Linköpings university 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. The Centre’s principal tools are high level research, advanced teaching and the organisation of specialist conferences and workshops. Work at the Centre 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 Norrköping 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), Hacettepe University (Turkey), Italian Institute of Technology in Pontedera, Jiangsu University (China), Manchester University (UK), University of Dundee (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), Universitat Rovira i Virgili (Spain), Zanjan University (Iran) and a number of well-known companies.

CONFERENCES AND WORKSHOPS

EuroEAP conference (10-11 June 2014)

Edwin Jager and his team organised the 4th EuroEAP conference at the Primurare Hotel in Linköping. Over 120 scientist from around the world participated in this two day event, discussing all aspects of electroactive polymers and their applications. The conference dinner was held at the Air Force Museum (Flygvapenmuseum). During the dinner, IFM researcher Prof Olle Inganäs received the ESNAM award for his contribution to the development of conducting polymer actuators.

Conference dinner at the Flygvapenmuseum.

Biosensors 2014 – Melbourne

Nine members of IFM travelled to Australia to chair and present to over 800 people at the 24th anniversary World Congress on Biosensors. In addition to poster and oral presentations, LiU had an exhibition stand with Acreo Swedish ICT AB. The next World Congress on Biosensors will be a little more accessible, since it will be held in Gothenburg in May 2016 www.biosensors-congress.elsevier.com/biosensors%202016.html
International Conference on Smart Materials and Surfaces, 26-28 August 2014, Bangkok, Thailand.

SMS was a 3-day event chaired by Ashutosh Tiwari, which was focused on the design, modification, characterisation and applications of smart and active surfaces and materials. There were 4 plenary talks, 8 invited talks, 48 oral presentations and 80 poster presentations.

Ashutosh was also Co-Chair of the Sweden-India workshop on Advanced Materials for Health and Energy, 30-31 August 2014, Indian Institute of Technology, Guwahati, India.

As part of the Pathoscreen project, Ass. Prof. Veli Cengiz Ozalp from the Istanbul Kemerburgaz University (Turkey) visited LiU to improve collaboration between the two universities. Similarly, Valerio Beni visited the Istanbul Kemerburgaz University and was invited to visit and present seminars at various other research centres including Gazi University (Ankara), Izmir Institute of Technology (Izmir) and the Turkish Standards Institute (Istanbul).

JOURNALS

Biosensor and Bioelectronics (Elsevier)

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. This year, the Impact Factor rose to an impressive all-time high of 6.451, making it the highest ranking research publication in the entire field of Analytical Chemistry, as defined by ISI, and also the top journal in both Electrochemistry and in Sensors. The team handled 3,100 submissions in 2014. [www.elsevier.com/locate/bios](http://www.elsevier.com/locate/bios)

Advanced Materials Letters

Ashutosh Tiwari is Editor-In-Chief of Advanced Materials Letters, published by VBRI Press. The journal has an Impact Factor 1.93 and handled 642 papers in 2014, with a rejection rate of 83.4%. [www.amlett.com](http://www.amlett.com)

BOOKS

Advanced Materials book series

Ashutosh Tiwari is Series Editor for the Advanced Materials book series published by Wiley-Scrivener (USA). Seven books were published in this series in 2014:

Biosensors: Fundamentals and Application

The first ever textbook on Biosensors was made available on open access by LiU Electronic Press following the reversion of rights to the book to Tony Turner by Oxford University Press. The full-text PDF can now be downloaded for free from: [http://urn.kb.se/resolve?urn=urn:nbn:se:liu:diva-92007](http://urn.kb.se/resolve?urn=urn:nbn:se:liu:diva-92007)

[www.ifm.liu.se/biosensors](http://www.ifm.liu.se/biosensors)

EXCHANGE VISITS
Linköping Initiative in Life Science Technologies (LIST)

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” (2009-2014). The missions of LIST have been 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. IFM has been the administratively responsible department of LIST and has during 2014 lent four of its staff members to work with the Center: Ingemar Lundström (chairman of the steering committee), Anthony Turner (member of the steering committee), Karin Enander (part time director), and Anke Suska (part time co-director).

During 2009-2014, LIST has supported selected research projects (in total 1 MSEK/year) at LiU. It has also been possible for LiU researchers to receive travel grants and support for arrangement of workshops, symposia and conferences. In 2014, LIST granted financial support to the following research projects:

- Imaging, modeling, and simulations of dynamic processes in the human brain. Main applicant: Maria Engström (IMH/CMIV)
- A novel implantable device for blood flow assessment after microsurgical reconstructions based on wireless energy and data transmission. Main applicant: Simon Farnebo (IKE)
- Health effects of resistance training on postmenopausal women. Main applicants: Mats Hammar (IKE) and Magnus Borga (IMT)
- Printed biosensors to monitor simultaneously multiple metabolites for sensitive, reliable and personalised management of diabetes. Main applicant: Martin Mak (IFM)
- In vitro modulation of heart cells beating: A novel technique toward developing a natural pacemaker. Main applicant: Mehrdad Rafat (IMT)
- Explore detecting bioluminescence with organic photodetectors for biosensing applications in HCT-116 colon cancer cells. Main applicant: Fengling Zhang (IFM)
- A personalized model for Type 2 diabetes patients. Main applicant: Gunnar Cedersund (IKE/IMT)

LIST arranges workshops and other events, mainly with the purpose to increase research interactions between LiU faculties but also to increase contacts between academia and industry. In April 2014, LIST co-arranged an “elevator pitch” session with NovaMedTech, where senior researchers within sensor science and representatives from a number of companies from the medical technology area were invited to give short presentations followed by mingling. LIST has also worked closely together with Grants Office, InnovationskontorETT and New Tools for Health in order to facilitate research and innovation within Life Science Technologies. During 2014, we co-arranged a number of information sessions on different national and international (Horizon 2020) funding opportunities.

“Welfare challenges” has been identified as a future profile area at LiU. During 2014, Karin Enander from LIST participated in the working group “Plats för välfärd”, commissioned by the Faculty of Health Sciences, with the task to arrive at a recommendation to the university board regarding how to implement this profile area within both research and education. In this context, LIST arranged a highly appreciated workshop in November 2014 together with the working groups “Plats för välfärd” and Äldres välfärd”, entitled “How can research at Linköping University address welfare challenges with respect to health and aging?”. In this workshop, almost 50 researchers from different faculties met to identify common projects addressing three selected welfare challenges.

http://www.liu.se/forskning/list
The aluminum–zinc-vacancy (AlZn-VZn) complex is identified as one of the dominant defects in Al-containing n-type ZnO after electron irradiation at room temperature with energies above 0.8 MeV. The complex is energetically favorable over the isolated VZn, binding more than 90% of the stable VZn's generated by the irradiation. It acts as a deep acceptor.

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 radial distributions in atherosclerosis for a better understanding of the role of reactive oxygen species (ROS) in atherosclerosis; (ii) imaging of radial 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.

**Ph.D. THESISES**

Shula Chen: “Excitonic Effects and Energy Upconversion in Bulk and Nanostructured ZnO”.

Yuttapoom Puttisong: “Room-temperature defect-engineered spin functionalities in Ga(In)NAs alloys”.

Axel Israelsson: “Chewing gum and human hair as retrospective dosimeters”.

Emelie Adolfsson: “Lithium formate EPR dosimetry for accurate measurements of absorbed dose in radiotherapy”.

**EDUCATION ACTIVITIES**

We have also been actively involved in undergraduate and graduate education. During 2014, the courses in “Semiconductor Technology” (TFYA39), “Perspectives on Physics” (TFFM12), “Experimental Physics” (TFFM08) were given.

**HIGHLIGHTS**


The aluminum–zinc-vacancy (AlZn-VZn) complex is identified as one of the dominant defects in Al-containing n-type ZnO after electron irradiation at room temperature with energies above 0.8 MeV. The complex is energetically favorable over the isolated VZn, binding more than 90% of the stable VZn’s generated by the irradiation. It acts as a deep acceptor.
with the (0/−) energy level located at approximately 1 eV above the valence band. Such a complex is concluded to be a defect of crucial and general importance that limits the n-type doping efficiency by complex formation with donors, thereby literally removing the donors, as well as by charge compensation.

**Stable and metastable Si negative-U centers in AlGaN and AlN**


EPR characterization of Si-doped AlGaN, 0.79 ≤ x ≤ 1.0, showed that Si already forms DX center with its negatively charged state E_D^- lying below the neutral charge state E_d. However, up to x ~ 0.83, the DX− state is still close to the neutral state E_D^- = E_d (EDX ~ 9 meV) and Si behaves rather similar to a shallow effective-mass donor. For x ≥ 0.84, two DX centers could be separately observed. For the stable DX1 center, the activation energy E_a = |EDX| increases drastically and linearly from ~71 meV in Al0.83Ga0.17N to ~240 meV in AlN. For the metastable DX2 center, the EDX level remains to be close to the neutral charge state E_d (EDX ~ 11 meV below E_d in AlN). The dependence of the EDX level of the stable DX1 center on the Al content explains well the sudden increase of the resistivity in Si-doped high-Al-content AlGaN reported by transport measurements.

**Imaging of reactive oxygen species in atherosclerotic plaques**


This study describes the development of an EPRI protocol and software for image reconstruction for the visualisation of oxidative stress in an ex vivo carotid atherosclerotic plaque. It was found that the areas with high EPRI signal intensity were found within or close to the cap in the area between the lumen and the plaque. Histopathology showed that these areas had presence of increased cellularity and frequent accumulations of foamy macrophages were interpreted as signs of activity. To the best of our knowledge no one has used diamagnetic cyclic hydroxylamines for EPRI imaging of oxidative stress as we demonstrated here.

**COLLABORATIONS**

About 30 research groups worldwide.
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Scientific Branch of Applied Physics

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Fernandez Del Rio, Lia et al. Polarizing properties and structural characteristics of the cuticle of the scarab Beetle Chrysina gloriosa In: Thin Solid Films, ISSN 0040-6090, E-ISSN 1879-2731, Vol. 571, no 3, 410-415
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