



# **INANO** REVIEW 2014/2015

#### Cover picture by former PhD student Casper Ibsen

#### At The Crystal Frontier

False color SEM image of warring  $CaCO_3$  polymorphs showing the transformation of vaterite (left) to the more stable calcite (right) on the surface of a hierarchical mineral tube grown from a gel-liquid interface.

Biannual review 2014-2015, published April 2015 iNANO – Interdisciplinary Nanoscience Center Science and Technology Aarhus University Gustav Wieds Vej 14 DK-8000 Aarhus C, Denmark

#### www.inano.au.dk

Editors: Maria Kragelund, Annette Wandahl and Peter Thostrup, iNANO and Hreinn Gudlaugsson, AU Communication. Photography: AU Photo Design: Aarhus University Printed in Denmark by Form og Farve

### CONTENT

- 5 MESSAGE FROM THE DIRECTOR
- 6 INANO HISTORY
- 8 THE FOUNDING FATHER PROF. FLEMMING BESENBACHER
- 10 INANO IN NUMBERS
- 12 AN INTERDISCIPLINARY CURRICULUM FOR NANOSCIENCE
- 14 GRADUATE STUDIES INANOSCHOOL
- 15 INANO RESEARCH GRAND CHALLENGES
- 16 MATERIALS INTRODUCTION
- 17 NANOFOOD INTRODUCTION
- 18 MEDICINE INTRODUCTION
- 20 INANO SENIOR RESEARCHERS
- 48 HIGHLIGHTS 2013 & 2014
- 50 INANO INFRASTRUCTURE PLATFORMS
- 51 CHARACTERIZATION
- 52 SYNTHESIS
- 53 NANOMODELLING
- 54 OVERVIEW OF INANO SENIOR RESEARCHERS
- 56 MESSAGE FROM THE CHAIRMAN
- 57 SPINOUT
- 59 INANO MANAGEMENT AND ADMINISTRATION



# I hope that the short presentations of our individual research groups

will facilitate the identification of overlaps in interests and complementary competences with new partners.

Jørgen Kjems

### MESSAGE FROM THE DIRECTOR



### INANO aims to be in the top 10 league of nanoscience centres in the world in terms of research.

Jørgen Kjems studied chemistry and physics at Aarhus University and received his PhD degree in the field of biostructural chemistry in 1989.

After being a postdoctoral fellow at Harvard Medical School, Boston, USA, 1989-1990 and at MIT, Cambridge, USA, 1990-1991, he returned to the Department for Molecular Biology, Aarhus University where he became an associate professor in 1994.

In 2003 he was appointed full professor in molecular biology. In 2010 he became the PI for a Lundbeck Centre, LUNA, which focuses on nanomedicine and the director of iNANO on January 1st, 2014.

He has published about 300 papers and has a H-factor of 52. His research competencies include non-coding RNA, gene regulation, self-assembled DNA nanostructures, nanotechnologies for nucleic acid delivery, bioimaging and tissue engineering.

It is with great pleasure that I present this first biannual report for the Interdisciplinary Nanoscience Center, iNANO. As of 1 January 2014 I took up the position as interim director of iNANO to continue in the footsteps of the former directors. I will continue the work to strengthen iNANO's position as a nanoscience center at the international forefront of research, education and innovation.

With the present report, we introduce a new concept which is meant to act as a presentation of iNANO as a whole to existing and potential partners in academia and industry, rather than a series of fragments. In particular, I hope that the short presentations of our individual research groups will facilitate the identification of overlaps in interests and complementary competences with new partners.

Underlying the new concept is our desire, as an organisation, to enter into mutually beneficial partnerships with other organisations. I feel that stronger ties to excellent organisations is one of the best ways to help researchers create strong teams for project applications and hopefully secure funding for groundbreaking research.

#### Organization

Since iNANO was inaugurated in 2002, the center has matured to a leading international nanoscience center with strong track records within education (BSc, MSc, and PhD level), research, technology transfer, collaboration with industry, innovation in the form of SME spin-outs. In this manner iNANO has demonstrated Scientific Social Responsibility. Today iNANO is a role model for large interdisciplinary centers (ICs) at Aarhus University (AU). Through the association of internationally strong interdisciplinary scientists from our partner departments, iNANO was designed from the outset to embrace studies at the nanoscale at the borderlines between traditional research disciplines. On this basis, iNANO serves its mission as an international spearhead within research, education, and innovation/industrial collaboration in the nanoscience area.

#### Strategic goals

iNANO aims to be in the top 10 league of nanoscience centres in the world in terms of research. To ensure such a position, we will enhance our research momentum through increased attraction of funding from Danish and European research foundations (public and private), participate in international research projects, form alliances with nanoscience centres at high-profile institutions, improve instrumental facilities/infrastructure to perform unique interdisciplinary research and attract young talented researchers to iNANO.

Finally, we will increase our focus on the rate of publication in high-impact journals. At the educational level iNANO will continue to internationalize the BSc and MSc educations by promoting increased student uptake and easing student exchange through the alignment of nanoscience educations with international partners.

### INANO HISTORY



#### 28 January 2002

 $(\mathbf{\Sigma})$ 

Inauguration of iNANO in the presence of the former Minister of Science Helge Sander, while Nobel Laureates Heinrich Rohrer and Professor Andreas Engel gave two scientific lectures.

••••••

August 2002 First group of Bachelor's degree students starts

.....

(>

(>

2007

The Board of Aarhus

University approves

the construction of the iNANO House

#### 2003 iNANOschool accepts its first PhD Student, Jan Kristian Jensen

(>

.....

2003 First major grant for interdisciplinary projects granted by the Danish Council for Independent Research



2007 First MSc in Nanoscience

.....

#### .....

24 September 2010 First iNANO PhD student, Karin Doolewerdt, graduates

.....



2011 Dorthe Ravnsbæk is recognized as the best PhD student in Europe with the European Young Researcher Award

January 2013 Official inauguration of the iNANO House





#### 6 August 2013

Prof. Niels Chr. Nielsen appointed as Dean of Science and Technology, Aarhus University Professors Troels Skrydstrup and Jørgen Kjems appointed interim directors of iNANO



.....



••••••

#### Summer 2005

The first students receive their BSc degrees in nanoscience

#### 2005

(>

Second major grant received for interdisciplinary projects from the Danish funding programme "Interdisciplinary Use of Nanotechnology, Biotechnology and Information and Communication Technology (NABIIT)"

••••••

#### 2005

(>)

First major EU grant awarded for a partnership with the "Frontiers" Network of Excellence

••••••

2007

 $\mathbf{O}$ 

iNANO students win the first annual Grundfos Challenge prize





January 2012 Founding director Prof. Flemming Besenbacher steps down as director of iNANO on the 10th anniversary of iNANO. Prof. Niels Chr. Nielsen



August 2012 The iNANO House is taken into use

2011 iNANO becomes role model for interdisciplinary centers at Aarhus University (Interdisciplinary Centers)

#### November 2011

Five iNANO Bachelor's degree students won the BIOMOD Grand Prize in the international **BIOMOD** Design Competition at Harvard University with their design of a new type of nanomedicine.

appointed as director of iNANO



1 January 2015 Prof. Jørgen Kjems appointed director of iNANO for a threeyear period.



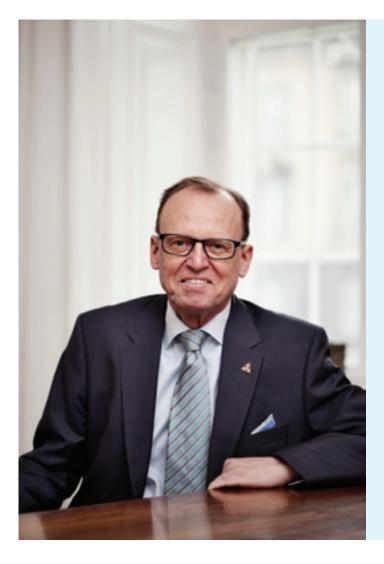
#### October 2014

New world-class research equipment comes into operation at iNANO. This includes a new high-flux SAXS instrument, new electron microscopes and a 950 MHz NMR.

------

### THE FOUNDING FATHER – PROF. FLEMMING BESENBACHER

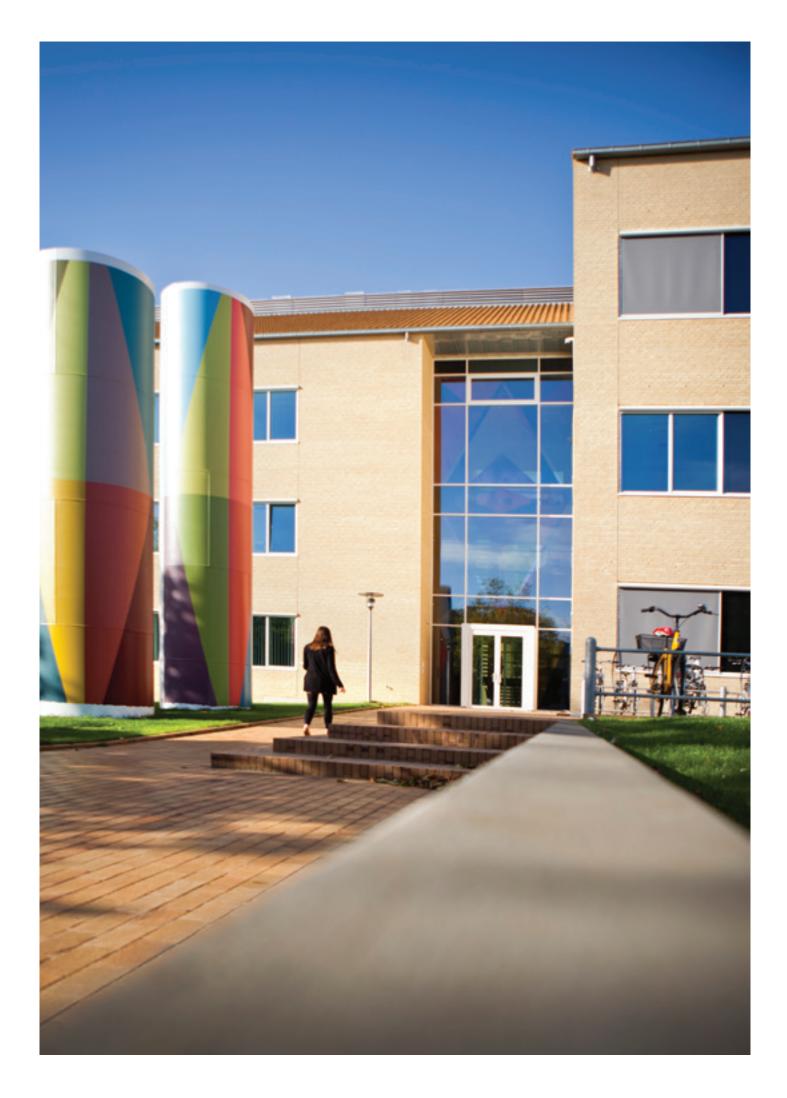




iNANO would not have come into existence were it not for its founding father. In 2001, Flemming Besenbacher was among the first to identify the new scientific trends embodied in nanoscience: interdisciplinarity and the vast possibilities in understanding and controlling the smallest of entities, the atoms. Hence the ideas behind the Interdisciplinary Nanoscience Center, iNANO, were born, and the center was inaugurated in January of 2002.

Initially, iNANO was meant to merely serve as the organization responsible for new interdisciplinary nanoscience BSc and MSc programs, but Flemming quickly identifies new opportunities in research. His visions and unparalleled ability to facilitate the setup of new research projects involving researchers from several traditional scientific disciplines made all the difference in the swift growth of iNANO. The third pillar of the iNANO mission, collaboration with industry, also quickly became very successful.

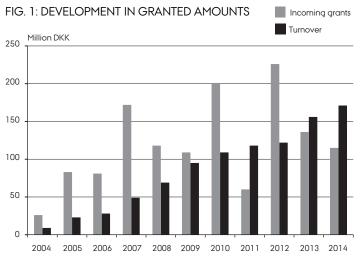
Flemming continued as the director of iNANO until 2012 when he was asked to take up the position as chairman of the Carlsberg Foundation and the Supervisory Board of Carlsberg Breweries. He retains a half-time professorship at Aarhus University and stays involved in research activities at iNANO.



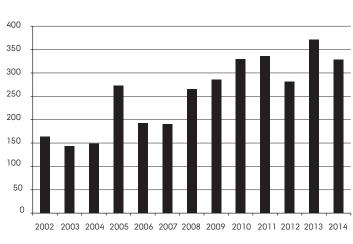
### **INANO IN NUMBERS**

Since its start in January 2002, iNANO has been one of the internationally leading nanoscience centers with strong track records within education (BSc, MSc, and PhD levels), research, technology transfer, industrial collaboration, and innovation in the form of spin-out companies. Today, thirteen years after its inauguration, iNANO is established as a collaborative interdisciplinary research center at Aarhus University. This would not be possible without different fields of expertise joining forces and strong support from the Faculty of Science and Technology and the University.

#### iNANO has attracted more than DKK 1300 Billion in external funding (Fig. 1)



### iNANO publishes around 300 papers per year (Fig. 2)



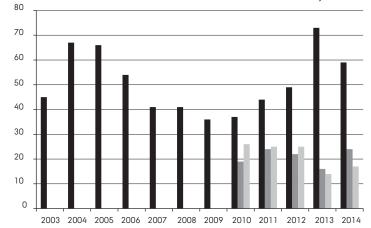
### Since 2002 iNANO has enrolled 40-70 Bachelor's students yearly (Fig. 3)

iNANO takes part in many industrial research collaborations, and importantly iNANO carries two well-run and highly recognised educational schools, including undergraduate studies on the BSc and MSc levels (Fig. 3)

#### FIG. 3: STUDENT INTAKE AND GRADUATES

FIG. 2: PUBLICATIONS





iNANO has a core of about 35 independent research groups, 11 satellite groups, and 14 collaborating medical groups involved in nanoscience research projects.

The high international level of the research activities is demonstrated by the fact that iNANO currently houses several Centers of Excellence sponsored by the Danish National Research Foundation, projects sponsored by the Danish Innovation Fund, projects sponsored by the Lundbeck Foundation, and numerous projects sponsored by the Danish Council for Independent Research as well as several EU projects and projects sponsored by other foundations.

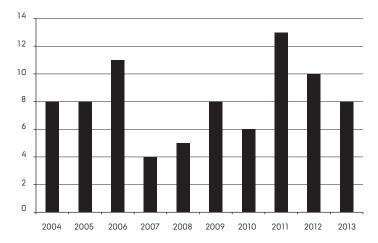
# PhD education with currently around 130 PhD students enrolled in the iNANO school graduate program (Fig. 4)

Approximately 40% of these have been recruited from abroad.

A large fraction of the iNANO MSc students continue as PhD students, internationally or in the iNANO PhD programme, iNANOschool.

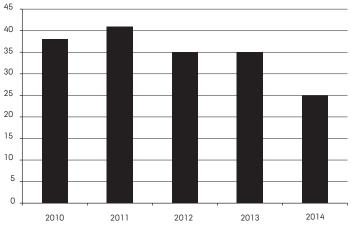
The total number of applied/issued iNANO patents reached 79 in 2013 (see Fig. 6)

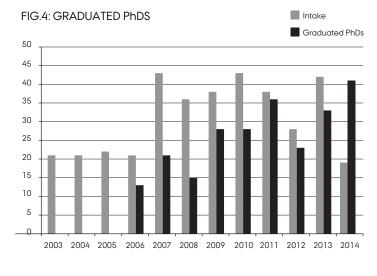
#### FIG.6: INANO PATENTS





shown in Fig 5.





The total number of distinguished lectures presented at iNANO is

### AN INTERDISCIPLINARY CURRICULUM FOR NANOSCIENCE

By Trolle Linderoth

Chairman of Educational board

Interdisciplinarity lies at the heart of nanoscience and nanotechnology. Many of the most groundbreaking developments take place at the boundaries between the traditional disciplines of physics, chemistry, molecular biology, and biology. This observation calls for an early introduction to all the core disciplines of nanoscience. At iNANO, we offer dedicated Bachelor's and Master's programmes in nanoscience where the goal of disciplinary breadth has been realized without sacrificing academic depth. Since its introduction in 2002 the nanoscience study programme has had an annual intake of 40-60 highly motivated and dedicated young students.

#### BACHELOR'S PROGRAMME

Students start the three-year Bachelor's programme by receiving fundamental interdisciplinary training in physics, chemistry, molecular biology and mathematics. The courses are often followed along with students from these core disciplines. In addition, several courses address issues specific to nanoscience. In the course "Introduction to Nanotechnology", the first-year students are introduced to key nano concepts such as scanning probe techniques and bottom-up/ top-down synthesis of nanostructures, e.g. involving an experimental exercise on DNA origami. The students also make a first contact with research groups at iNANO through a two-week project. In subsequent courses more advanced experimental exercises and an extensive project are carried out. In "Nanocharacterisation" the fundamental knowledge acquired in the first years of study is applied towards an understanding of key characterisation techniques and problems. Elective course modules during the third year of study allow finetuning of the course programme to the particular interest of the individual students. The Bachelor's degree programme is concluded by an individual Bachelor's project carried out in the research groups of iNANO. An extra-curricular program "iNANO Talent" caters to the needs of the most skilled and dedicated students by offering modules on innovative uses of nanotechnology as well as the possibility of internships in research groups and industrial partners of iNANO.

#### MASTER'S PROGRAMME

During the two-year Master's programme, the nanoscience students specialize in either nanophysics, nanochemistry, or molecular biology. Here they follow course programmes developed through individual counselling and can choose from Master's courses offered by iNANO such as "Bio-Nanotechnology", "Current Nanoscience", "Nanomedicine", or "Science-based Innovation and Entrepreneurship", as well as from a large suite of courses in the course catalogue of the Faculty of Science and Technology. In the compulsory "Student's Colloquium" the students train their communication skills by studying and presenting a subject of their own choice to fellow students. The specialisation courses followed during the fourth year of study enable the students to commence their Master's project or alternatively to seek admittance to the PhD programme of iNANOschool.

#### SINO-DANISH NANOSCIENCE MASTER'S DEGREE

As an additional educational activity, iNANO is partner in a Sino-Danish Nanoscience Master's programme offered in Beijing by the Sino-Danish Center for Education and Research (SDC) in collaboration with the Chinese Academy of Sciences (CAS). The English-taught nanoscience Master's degree is open to both Danish and Chinese students and has been developed in a joint effort with the Nanoscience Center at Copenhagen University and the National Center for Nanoscience and Technology (NCNST) in Beijing. iNANO provides courses in nanocharacterisation, bio-nanotechnology and nanoenergy materials, which are taught jointly by Danish and Chinese teachers.



#### MASTER'S PROJECT IN NANOTECHNOLOGY

Specialisation	Specialisation
	opecialisation
Specialisation	Specialisation
Specialisation	Specialisation
Specialisation	Specialisation
Elective	Elective
Molecular structure	Elective
Nanocharacterisation	Elective
Fourier analysis	Elective
Statistics and data analysis	Advanced molecular biology
Linear algebra	Numerical physics
Theory of science (Nano)	General molecular biology
Physical chemistry	General biochemistry
Organic chemistry	Introduction to nanoscience
	General biology
the environment of the environment of the second states of	Calculus 2
Inorganic chemistry	Culculus z
	Specialisation Specialisation Elective Molecular structure Nanocharacterisation Fourier analysis Statistics and data analysis Linear algebra Theory of science (Nano) Physical chemistry Organic chemistry

Course programme for the interdisciplinary Bachelor's and Master's degrees in nanoscience offered at iNANO.

physics courses

chemistry courses

molecular biology courses

mathematics/computer science courses

compulsory nanoscience courses selected elective courses specialisation modules

Each academic year (starting from the bottom) is divided into four 7-week quarters and three courses are followed in each quarter.



### **GRADUATE STUDIES** – INANOSCHOOL

www.iNANOschool.au.dk

**By Duncan Sutherland** Head of iNANOschool

With currently 130 PhD students enrolled, iNANOschool is a graduate school of international stature. A range of specialized graduate courses are offered alongside access to highly advanced research facilities. This combination makes iNANOschool a nexus of interdisciplinary competences in nanoscience and nanotechnology at the highest international level.

More than ten years after the establishment of iNANOschool, the main objectives remain the same. The major driving force is the education of highly qualified, internationally competitive PhDs with a broad range of interdisciplinary competences within nanoscience and nanotechnology. The research areas of iNANO and iNANOschool are highly integrated as well as truly interdisciplinary and cover at present such diverse research fields as:

- functional nanomaterials,
- nanoenergy materials,
- nanomedicine,
- self-assembled molecular nanostructures,
- nanofood,
- · nanophotonics and -electronics,
- nanotoxicology and nanoethics.

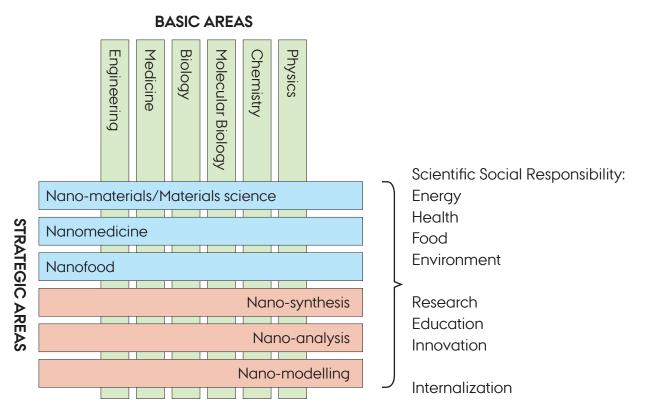
Many of the PhD research projects involve more than one research group and in frequent cases also industrial research laboratories. Overall, the research activities are at the international forefront of science and serve as an ideal framework for education and industrial collaboration. In addition to research, iNANOschool offers several PhD courses within nanoscience and nanotechnology and provides access to facilities for and supervision of approximately 130 PhD students. During 2013-2014, 61 new PhD students were enrolled in iNANOschool and 74 PhD students completed their PhD studies.

In addition to the focused PhD courses, activities include a major annual meeting, an autumn school, student networks, and initiatives to promote exchange with international institutions.

### **INANO RESEARCH** – GRAND CHALLENGES

iNANO research combines competences within traditional disciplines (vertical bars in the figure) through interdisciplinary research focusing on structures and processes at the nanoscale. The impetus behind our research strategy is to instil a strong sense of scientific social responsibility (see P. Krogsgaard-Larsen, P. Thostrup, and F. Besenbacher (2011), Editorial: Scientific Social Responsibility: A Call to Arms. Angew. Chem. Int. Ed., 50, 10738) to address Grand Challenges into iNANO researchers, which should act to direct their choice of fundamental research projects and collaborative partners. We have established groupings within three key strategic research areas (nanomaterials, nanomedicine, and nanofood), exploiting three unique iNANO infrastructure platforms (nanosynthesis, nanoanalysis, and nanomodelling) (horizontal bars in the figure). These focus areas, each of which contain many separate research themes, are defined from their interdisciplinarity and potential to contribute to meeting the Grand Challenges of our time; many of these challenges seek solutions with components of nanoscience and nanotechnology. Furthermore, these Grand Challenges have also directed political focus to select strategic areas, which in turn will be the foci of future funding opportunities.

This does not imply that iNANO researchers do not conduct basic research. On the contrary, our experience shows that there is no conflict between performing basic and strategic research; one acts to stimulate the other and in the ideal case, research in a given research area lies on the entire continuum between the two extremes.



iNANO strategic research areas and infrastructure platforms exploiting competences in basic research disciplines

### MATERIALS - INTRODUCTION

#### STRATEGIC AREA 1: NANOMATERIALS

iNANO has many strong and expanding activities within nanomaterials, particularly in these areas: chemical and physical surface modification, catalysis, nanoenergy materials such as hydrogen storage, thermoelectrics, biofuel conversion, photovoltaics, semiconductor physics, nanocomposites, self-assembled nanostructures, bio-mineralization, and fiber materials. Within several of these topics, iNANO is at the absolute forefront internationally, such as heterogeneous catalysis, self-assembled DNA nanostructures, novel construction materials, and thermoelectric materials.

#### BIODIESEL

High-pressure conversion of wet biomass to transportation fuels is a novel technology with overwhelming environmental and economic advantages. The Catliq® process has been developed, patented, and commercialized by Steeper A/S. In a range of collaborative projects, iNANO carries out laboratory scale studies of the process using a specially designed supercritical gold reactor. Furthermore, iNANO devotes extensive efforts to the development and test of new nanocatalysts and the development of methods for efficient characterization of the oil product.

#### ENERGY STORAGE

The most critical obstacle in the development of hydrogen technology is the storage of hydrogen. The problem is easily seen by comparing the energy to volume ratio for gaseous hydrogen (3.0MJ/L) to that of conventional gasoline (32.0MJ/L). So how can one store hydrogen for use in, e.g. cars? Possible solutions are: the use of liquid hydrogen (8.5MJ/L), compressed hydrogen or to store hydrogen in solid metallic hydrides (e.g. MgH2, LaNi5H6 or TiFeH2). iNANO focuses on the surface (nano)catalysis and the storage of hydrogen using complex metallic hydrides. The latter involves studying synthesis as well as catalytic properties of metallic hydrides.

#### **FUEL CELLS**

Modern society is founded upon energy that is mainly produced by the burning of fossil fuels. Besides its unacceptable influence on our climate, this resource will eventually become exhausted. Thus, there is a growing need for alternative energy, e.g. hydrogen, which is available in large quantities. To exploit the energy stored in hydrogen, it is necessary to find non-polluting ways to manufacture hydrogen and develop fuel cells which transform H2 and O2 into H2O.

#### NANOCATALYSIS

Catalysis is of vital importance to our society. The availability of plentiful and inexpensive chemicals relies on industrial catalytic processes. Without these processes, it would be impossible to maintain the current living standard for more than a minute fraction of the present human population. Catalysis is also the key to the development of novel technologies for environmental protection and the production and distribution of sustainable energy.

iNANO is at the forefront of research in nanocatalysis, which is expected to revolutionize the way catalysts are developed and prepared. The traditional empirical way of discovering a catalyst has been through 'trial-and-error' methods. However, with the ability to design and characterize new nanomaterials and, thereby, predict their catalytic capabilities from first principles, a new era for catalyst development is within reach.

#### THERMOELECTRIC MATERIALS

Thermoelectric materials are functional materials, which are attracting huge attention due to their dual capability of electrical-thermal energy conversion. Thus, thermoelectric materials can convert heat to electrical energy or be used for cooling. Devices built from thermoelectric materials exhibit very high reliability without noise or vibration because there are no mechanical moving parts. They are portable, scalable and light-weight. iNANO research in this area is internationally renowned and is currently being commercialized.

#### SOLAR CELLS

The current market for commercial solar cells is dominated by 1st generation monocrystalline and multicrystalline Si-solar cells. One drawback of these solar cells is that relatively thick (~300-400  $\mu$ m) layers of Si are needed, and the electrical quality of this Si has to be very high in order to ensure a sufficient solar power conversion efficiency. As a consequence the price of energy produced by modern commercial Si-solar cells is still not competitive, although substantial technological progress and cost reductions are seen these years. At iNANO, we work to develop thin-film Si-solar cells and thin-film photovoltaics for roll-to-roll fabrication, which are made of thin Si layers (~1-2  $\mu$ m) and can be produced substantially cheaper due to the smaller amount of Si used.

### NANOFOOD INTRODUCTION

In recent years rapid advancements in nanosciences and nanotechnologies have opened up for food related applications offering a wide range of possible benefits to the consumer. These benefits include a reduction in the use of agrochemicals such as pesticides, antibiotics, veterinary medicines, and less harmful chemical residues in food.

The reduction in the use of food preservatives, salt, fat and surfactants in food products and the development of new or improved flavours, other textures and mouth feels have occured through nanoscale processing of foodstuffs. Nanoformulations can also improve the uptake, absorption, and bioavailability of nutrients and supplements in the body compared to our usual or traditional food.

Nanotechnology-derived polymer composites offer new lightweight and stronger food packaging materials that can keep food products secure during transportation, fresh for longer time during storage, and more hygienic (safe from microbial pathogens).

Food quality nanosensors, integrated with packaging, may increase the shelf life of food by detecting spoilage bacteria or the loss of food nutrients, possibly releasing antimicrobials, flavours, colours or nutritional supplements in response. Antibacterial nanocoatings on food preparation surfaces can also help maintain hygiene during food processing.

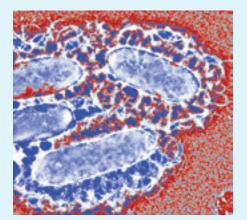
However, despite the projected benefits, the current level of nanotechnology applications in food and related sectors is still very new and the vast majority of new developments are still at the R&D or near-market level.

#### SAFETY

Any concerns over consumer safety mainly relate to long-term use, or new and unforeseen harmful effects of exposure to nanomaterials. Nano-additives in food are also likely to undergo various transformations in food and in the GI-tract due to agglomeration, aggregation, binding with other food components, and reaction with stomach acid, enzymes, and other biotransformation in the body. Such transformations may lead to nanomaterials losing their 'nano' characteristics.

There is currently very little known of the nature or impact of biotransformations on the safety of nano-food products.

### NANOFOOD AT AU





Nanofood at AU includes research into enzyme encapsulation and immobilization strategies, sensors, novel ingredients, protein digestive systems of animals and plants, milk protein biophysics, enzyme modelling, antifouling surfaces, antimicrobial compounds, oral microbiology, as well as nutrigenomics.

iNANO seeks to markedly expand activities in this area and to foster collaboration with new AU research groups and international as well as national key players in the area of nanoscience with relevance to food and nutrition. The research involves a high level of industry collaboration, as currently demonstrated by iNANO's joint research programs with, e.g. **Arla**, **Danisco**, and **Nestlé**.

By Gunna Christiansen and Brian Vad: False color TEM image of *pseudomonas* bacteria that produce amyloids as a part of a biofilm network.

### **MEDICINE** INTRODUCTION

#### INTRODUCTION

Nanomedicine is the medical application of nanotechnology. In the future nanomedicine will provide important tools for understanding, diagnosing and treating diseases. By exploiting novel physical, chemical and biological properties of materials at the nanometer scale, nanomedicine will provide targeted, site specific therapeutics with reduced adverse effects, drug delivery systems and pharmaceutics, novel imaging methods for the early diagnosis of diseases, and novel implant materials that support tissue regeneration processes. Nanomedicine ranges from the medical applications of nanomaterials, to nanoelectronic biosensors, and possible future applications of molecular nanotechnology. Current challenges in nanomedicine involve understanding the issues related to toxicity and environmental impact of nanoscale materials.

#### DRUG DELIVERY AND DESIGN

#### Drug delivery

Nanomedical approaches to drug delivery center on the development of nanoscale particles or molecules for the improvement of drug bioavailability. Bioavailability refers to the presence of drug molecules where they are needed in the body and where they will do the most good. Drug delivery focuses on maximizing bioavailability both at specific places in the body and over a period of time. The effectiveness of a drug is determined by its ability to migrate through the body and reach diseased tissue (and if necessary enter cells) in therapeutically relevant levels.

The drug delivery activities at iNANO cover both nanoparticle delivery systems (polymeric systems, liposomes and layer-by-layer nanoparticles) and polymer hydrogel thin films. The inclusion of "biological triggers" into the nanocarrier design is used for the modulation of cellular nucleic acid trafficking and increased target interaction.

#### Drug design

Structure at the atomic level equals function in biology and medicine. Drug molecules must fit into their receptors as a hand in a glove to exercise their therapeutic effect, and medicines should only interact with specific targets to avoid undesired side effects. One way to achieve this is to determine the three-dimensional atomic structures of drug receptors and analyze their interaction with a drug.

#### DIAGNOSTICS

Studies of nanotools for diagnostic purposes encompass the development of biomedical imaging technology and sensor technology. Generally speaking, a sensor is a device capable of recognizing a specific chemical species and 'signaling' the presence, activity or concentration of that species in solution through chemical changes. A 'transducer' converts the chemical signal (akin to the catalytic activity of a specific biomolecule) into a quantifiable signal (such as a change in color or intensity) with a defined sensitivity. When the sensing is based on biomolecular recognition, it is called a biosensor. There are various types of biosensors, classified according to the technique used in signaling transduction biosensors.

Non-invasive studies of disease processes and their underlying biomolecular interactions are becoming the backbone of diagnostic imaging as well as in connection with identifying new drug targets, optimizing the distribution of drug candidates, and individualizing the therapy of humans. Hence, the development of novel imaging modalities of disease progression, drug biodistribution, and therapeutic efficacy is crucial to treatment as well as innovative drug development and testing. In parallel, nanoscience research has revolutionized the prospects of engineering customized 'vehicles' for targeting specific tissue properties by bio-imaging and indeed for the development of advanced therapies.

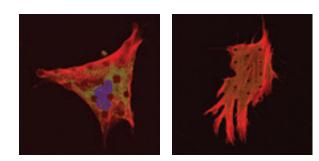
#### TISSUE ENGINEERING AND BIOCOMPATIBLE MATERIALS

Nanotechnology may be able to help reproduce or repair damaged tissue. "Tissue engineering" makes use of artificially stimulated cell proliferation by using suitable nanomaterial-based scaffolds and growth factors. For example, bones could be regrown on carbon nanotube scaffolds. In the future tissue engineering might replace today's conventional treatments such as organ transplants or artificial implants. Advanced forms of tissue engineering may lead to life extension. The artificial regeneration of tissue, whether ex vivo or in vivo, and the biocompatibility of artificial material in the body depends on extremely complicated cellular processes and microenvironment responses.

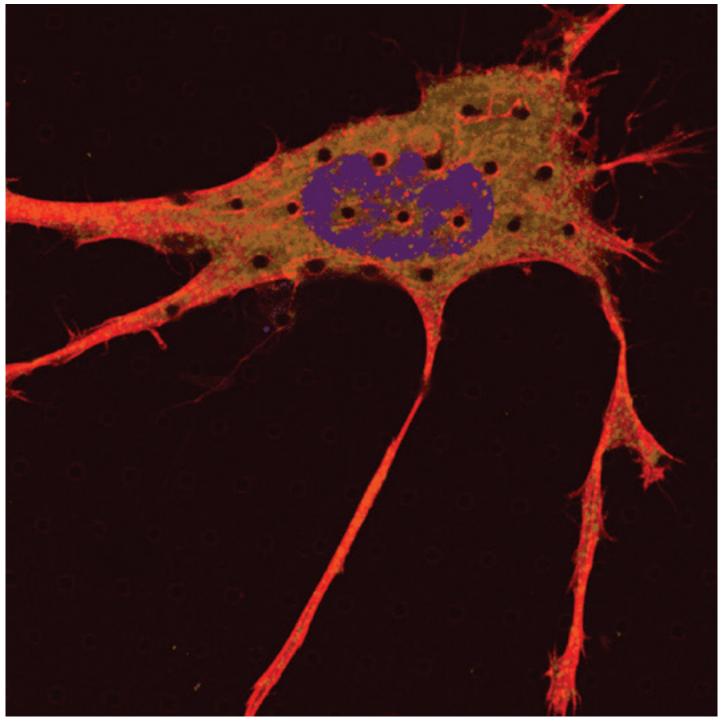
Tissue engineering and the development of biocompatible materials at the nanoscale aim at providing control over tissue cells and guide them to collaborate in a desired manner.

Within a few milliseconds after an implant is inserted into the body, a biolayer consisting of water, proteins, and other biomolecules from the physiological liquid is formed on the implant surface. The chemical and topographical properties of the implant surface strongly influence the properties of the layer and this influence needs to be understood and controlled in order to optimize biocompatibility. Likewise, maintaining and controlling stem cell differentiation is the key to potential treatment of chronic degenerative disease. Nanotechnology approaches to generate defined cell populations specific to some diseases are being developed, and the resultant cellular systems are tested in in vitro and in in vivo disease models.

For instance, studies of regenerative medicine at iNANO involve the construction of nanostructured scaffolds that are biodegradable and functionalized with structures and drugs which tune the cellular responses in the surroundings to regenerate the desired tissue.



By former Master's student Jonas Bøgh Pedersen: Digitially color enhanced confocal microscopy images of human dental pulp stem cells proliferating on a structured array of micropillars of a PDMS substrate.



# INANO SENIOR RESEARCHERS

CURRENTLY INANO CONSISTS OF





Postdocs

### STRUCTURAL BIOLOGY OF FUNCTIONAL AMYLOIDS:

IN FIBRIL FORMATION, BIOFILMS AND INFECTION

> NMR-Supported Structural Biology Group, Ümit Akbey, PhD in NMR spectroscopy, Assistant Professor

We aim to determine the first atomic-resolution structure of a functional amyloid, which is a non-soluble and non-crystalline solid protein aggregate. Functional amyloids are a new type of aggregated proteins with distinct biological functions, and as a result differ from other disease-related protein fibrils (such as  $\alpha$ -synuclein in Parkinson's disease). However, since they support the integrity of biofilms and make an infection difficult to treat, they are drug targets, just like other components of bacterial biofilms (80 % of human bacterial infections are due to biofilm formation).

We use advanced solid-state nuclear magnetic resonance (ssNMR) in combination with hyperpolarization for sensitivity enhancement and recombinant protein production. ssNMR is one of the few tech-



niques capable of providing atomic resolution, and has proven very powerful for obtaining insight into the structural biology of insoluble proteins. The determination of the unknown structures of amyloid fibrils is an important step towards understanding protein aggregation in function and disease, and thus plays a key role in the search for possible medical treatment and clarification of the protein folding/ misfolding paradigm.

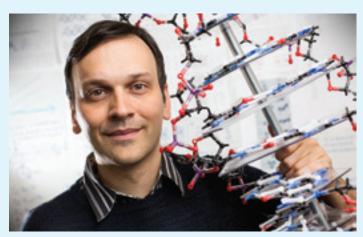
Our research is highly interdisciplinary and is performed in collaboration with researchers from iNANO and abroad, as well as industrial partners, for understanding and treatment of functional amyloid related diseases. Funding obtained from Denmark and EU (via DFF MOBILEX and AIAS COFUND) ensures ample progress of the project.

### **DESIGNING BIOMOLECULES** TO CREATE NANOSCALE DEVICES

Biodesign Group, Ebbe Sloth Andersen, PhD in molecular biology, Assistant Professor

Our research aims at understanding the fundamental principles for how biomolecules fold into unique and functional shapes and at using this insight to guide the design of novel nanoscale devices for technological applications.

Biomolecules can self-assemble into unique three-dimensional (3D) shapes determined by their sequence of residues. This causal relationship allows us to design the shape of biomolecules by programming their sequence. Our design process starts by investigating the atomic structure of nature's biomolecules from which we extract structural modules and invent new ways of combining them into a defined 3D shape. In a second step, we use computer algorithms that take into account the physical properties and folding kinetics of the molecules to design their sequence. The sequences are then chemically synthesized and



used in self-assembly experiments followed by investigation of their 3D structure and properties by biophysical characterization techniques.

Our research group has been involved in developing the DNA origami method to create 3D nanomechanical devices such as the DNA origami box and we are further developing DNA origami devices for applications in biosensing, enzymatic control and drug delivery. Recently, we have invented the RNA origami method that allows nanostructures to be enzymatically synthesized and possibly expressed in cells. We aim to use this new technology for synthetic biology purposes as intracellular sensors and as scaffolds for biosynthesis pathways of relevance to the biotechnology industry.

### "TEACHING" **SEMICONDUCTOR MATERIALS** NEW MANNERS

#### Semiconductor Group,

Peter Balling, PhD in physics, Professor

There are many examples of how the ability to control a material on the nanoscale opens up for entirely new properties and applications. In the Semiconductor Group this approach is employed to produce new functional materials and characterize them with respect to their technological applications and their ability to answer fundamental questions. For this purpose, we have built up a laboratory with a broad range of equipment for thin film synthesis, and for structural, optical and electrical characterizations.

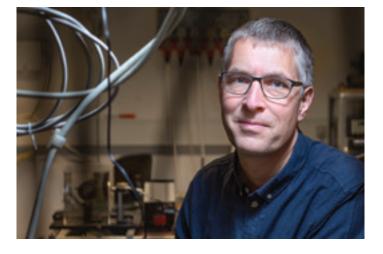
The growth of high-quality thin epitaxial layers of group-IV semiconductors using molecular beam epitaxy (MBE) has been one of our core activities for many years. We are presently using this facility to grow thin expitaxial Si layers with embedded Ge or -Sn nanocrystals; this project is carried out in collaboration with Dr. Brian Julsgaard (for a detailed description of these activities, see page 34). Another major MBE activity is to develop new growth procedures for high quality epitaxial GaN layers on (111)-oriented Si substrates. GaN on Si substrates is considered one of the future materials for high power devices, but their different material properties make the epitaxial growth a challenge.

Si-thin film solar cells with functionalized back reflectors represent another active research area in the Semiconductor Group. We investigate amorphous, nano/microcrystalline, as well as crystalline solar cells, and common to all of these is that a large part of the photons from the sun is not absorbed in the thin film solar cell, either because their optical path lengths are longer than the thickness of the solar cell, or because they have too low energy to create an electron-hole pair. We investigate nano-optical methods for the development of efficient back reflectors capable of "tuning" the color spectrum of the sun, e.g. by upconverting the infrared part of the solar spectrum to a wavelength which can contribute to new photocurrent.

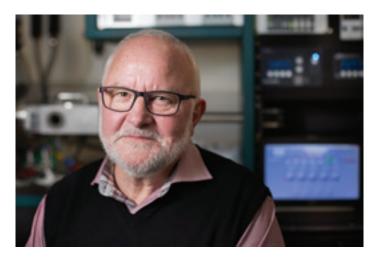
The Semiconductor Group has a long experience in investigating the influence of structural defects in crystalline semiconductors on their electrical and optical characteristics. These methods are still being pursued in joint projects with producers of silicon such as Topsil Semiconductors Materials A/S and Elkem Solar.

The recent affiliation of Peter Balling to the Semiconductor Group has opened up for new activities employing ultrashort-pulse lasers for both advanced optical characterization and for new laser-based material-processing techniques.

Many of our projects involve both applied and fundamental aspects, and this has turned out to be a very fruitful playground for the academic developments. Most of the projects involve collaborations with academic and industry partners from Denmark and abroad.



Semiconductor Group, Arne Nylandsted Larsen, Dr.scient., Professor



### **DEFENDING HUMANS AND PIGS** AGAINST PATHOGENIC BACTERIA

Animal Proteomics Group, Emøke Bendixen, PhD in molecular biology, Associate Professor

Our research aims to describe the molecular crosstalk that takes place when bacteria infect their host. This knowledge is essential for reducing the need for antibiotics in farm animal production, and hereby combating the explosive increase in multi-resistant bacteria, which currently presents a massive threat to public health. Our research in pig models is translated to improve our understanding of human immunology and defense against pathogens. This comparison is important because pig and man share many common pathogens due to our long history of close contact and co-evolution.

We use mass spectrometry (MS) to study how genetic variation affects adhesion molecules and immunological pathways. The MS technology makes it possible to analyze changes directly within the functional protein networks of cells, hence closely reflecting protein function within the living organism. We also study 16sRNA based



metagenomes from gut samples to achieve information about which specific bacterial species are present in the animal gut. In combination, these data can explain how specific bacteria adhere to specific receptors, and how their adherence is controlled by the individual genetic signatures of individual animals. We collaborate with Prof. N. Packer (Sydney) to characterize how specific carbohydrate molecules allow the gut cells to select and sort which bacteria may inhabit their host, and with Profs. R. Beynon (U of Liverpool) and R. Moritz (ISB, Seattle) to advance the MS methods we use.

### **LEARNING MATERIALS CHEMISTRY** FROM BIOLOGY

Biological and Bioinspired Materials Group, Henrik Birkedal, PhD in physics, Associate Professor

We study the structure and properties of biological materials and perform syntheses of bioinspired materials using lessons learnt from biology.

We study biological materials to understand the connection between their structure and function. Many of these hierarchical materials contain inorganic crystals organized in 3D within an organic matrix. We study bone and a model organism for underwater attachment, the bivalve Anomia simplex that unlike other mussels uses a mineralized anchor for attachment. We use a wide range of experimental approaches. X-ray based scattering, diffraction and imaging methods form the center piece of our experimental platform, and we are avid users of synchrotron radiation.



We make several types of bioinspired materials using green reactions in liquid water. Bioinspired crystallization is used to make nanocrystalline phosphates, oxides and other materials. As an essential aspect of this effort, we study crystallization mechanisms using in situ X-ray scattering and diffraction. We employ coordination chemistry to make self-healing hydrogel materials whose properties are tuned by controlling the balance between covalent network formation and coordination chemistry crosslinking. This allows us to obtain self-healing materials with controlled properties.

Aspects of our work have an applied focus and involve collaborations with academic, researchers at hospitals and/or industry partners.

### CAUGHT IN THE ACT: INDIVIDUAL BIOMOLECULES AT WORK

Biophotonics and Nanoscale Biophysics Group, Victoria Birkedal, PhD in physics, Associate Professor



Our research focuses on elucidating the structure and dynamics of nucleic acids and their interaction with proteins, which is essential for understanding the machinery of life as well as diseases. Nucleic acids are able to fold into astounding functional structures of which we seek to achieve a molecular understanding and control.

We study the folding and dynamics of a number of nucleic acid structures of telomeres, in the HIV genome, and structures relevant to DNA nanotechnology. Specific structures are visualized and studied with fluorescence and Förster resonance energy transfer (FRET) spectroscopy and single molecule microscopy. Studies at the single molecule level allow us to obtain much deeper and detailed insights into the nanoscale machinery of biological systems and provide information on population heterogeneities unavailable with traditional ensemble biochemical and biophysical studies. By using and making further development of the single molecule FRET microscopy, we are able to obtain exciting information on the structure, conformational dynamics and kinetics of nucleic acid molecules under physiologically relevant conditions.

Many of our projects involve the use of light to obtain structural dynamics information of biological relevance. We have recently started a new project in which we use biomolecules to build systems for photonic applications.

MATERIALS CHEMISTRY UNDER EXTREME CONDITIONS

> High Pressure Group, Martin Bremholm, PhD in chemistry, Assistant Professor

High pressure is a powerful approach to manipulate and study the atomic interactions in materials. We have established the first Danish lab that performs both synthesis and crystallography at extreme pressure and use these new tools for the synthesis of novel compounds and structure-property studies.

Activities in our home-lab are centered on synthesis and crystal growth followed by characterization of the crystal structures and physical properties. The facilities include single-crystal X-ray diffractometers compatible with small diamond cells that fit in a hand and the huge press that allows for syntheses of bulk samples at up to 20 GPa and 2000 K. In many cases compounds can be quenched to ambient conditions, similar to how diamonds are created in the Earth, but we do it in hours.



We study the structure and properties of materials with interesting electronic properties, such as multiferroics, superconductors and topological insulators. In many cases the compression leads to structural or electronic phase transition. We mainly perform structural studies at international synchrotron facilities using diamond cells under extreme conditions, 100 GPa and laser heating to 2500 K. X-ray crystallography is the principal diagnostic, but several other techniques can be used as diamonds are transparent to optical light and x-rays.

Many projects include collaborations with groups from physics/ nanoscience who perform theoretical calculations and advanced experimental characterization such as ARPES and STM/STS.

### THE ELECTROSPUN REGENERATIVE MEDICINE

ElectroMed Group, Menglin Chen, PhD in chemistry, Assistant Professor

The scientific significance of our research will be the creation of novel electrospun regenerative medicine that mimics the complexity of the nanocomposite nature of the extracellular matrix (ECM) to its closest, in order to direct cell reorganization for tissue regeneration.

Electrospinning is a versatile top down technique that utilizes high voltage electric fields to generate continuous nanofibers from virtually any polymers, composites or supramolecules that entangle in the same manner as polymers. This approach becomes particularly powerful when remarkable features such as very large surface area to volume ratio are combined with unique chemical, physical, and biological functionalization with ease and control. The resemblance of ECM fibrillar structures led us to explore novel regenerative medicines that not only provide biomimetic nanostructures for homing cells, but also sufficient approachable biological cues that may synergistically promote regeneration.

Our current research involves the morphology control of the nanofibers, the delivery of growth factors, anti-inflammatory drugs or other cell signaling molecules to stem cells, and bioactive on-demand delivery strategies.

Our projects involve collaborations with academic and industry partners with focus on specific applications, such as the development of meshs for pelvic floor repair and the development of scaffolds for vascularization and disc regenerations.

### SMART NANOMAGNETS

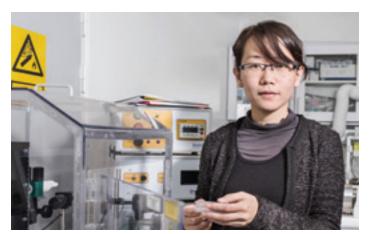
Magnetic Materials, Mogens Christensen, PhD in chemistry, Associate Professor

Our goal is to obtain insight into magnetic materials over many length scales ranging from the atomic scale via the nanometer to macroscopic length scales. Understanding all length scales of permanent magnets is paramount in the quest for the development and design of more efficient permanent magnets without the use of scarce raw materials such as rare earth elements.

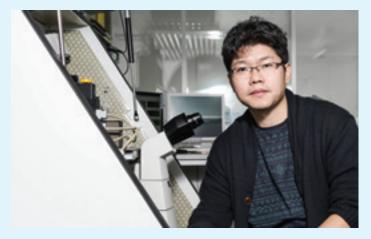
Different synthetic approaches are applied to prepare magnetic nanoparticles with specific atomic structures. Simultaneously with the preparation of the atomic structure, we also use synthesis conditions that allow us to control the size and shape of the magnetic nanoparticles. In the characterization process we use neutron and X-ray powder diffraction techniques, which allow us to elucidate not only the atomic structure and shape of the nanoparticles, but also the magnetic structure at the atomic level. Magnetic force microscopy is used to study the magnetic properties of individual nanoparticles, while vibration sample magnometry is used for macroscopic investigations. To improve the magnetic performance, the nanomagnets must be aligned with respect to each other on the micrometer scale. Understanding and controlling all length scales of smart nanomagnets are essential to improve the magnetic properties.

Our projects span broadly from fundamental research at the most advanced international neutron and synchrotron facilities to collaboration with industrial partners, who potentially can use our magnets in new products.





**BEYOND STRUCTURES POWERED BY** AFM-BASED DYNAMIC QUANTITATIVE IMAGING



**BioSPM Group,** Mingdong Dong, PhD in applied physics, Associate Professor

Our research interests focus on the development of a surface sensitive technique, Atomic Force Microscopy (AFM), to study molecular structures as well as novel functional nanomaterials for biological applications.

With more than 10 years of experience in scanning probe microscope, we have developed a novel AFM-based platform for quantitative nanomechanical imaging methods, including microsecond force spectroscopy, microsecond single-molecule recognition spectroscopy, etc. These "advanced" AFM techniques with sub-molecular resolution and high-scanning speed have been applied to study dynamic and physical properties of biological systems. One of the topics is to monitor abnormal conformational transitions of proteins associated with amyloid-related diseases by combining imaging and force microscopy. Detailed information on the morphology and mechanical properties of the peptides throughout the aggregation process could contribute to the development of treatment methods for a variety of diseases.

Many projects involve collaborations with international leading companies such as Lundbeck A/S, Novo Nordisk A/S, DuPont Danisco, Danish Technological Institute, Carlsberg A/S, and Bruker USA. These industry collaborations enable us to extend our established fundamental academic platform to applied technology.

### CONSIDERING **CARBON DIOXIDE** AS A FRIEND

Organic Surface Chemistry Group, Kim Daasbjerg, PhD in organic electrochemistry and dr.scient., Professor

The goal of our research is to develop unique methods for converting carbon dioxide into high value chemical compounds. This will be accomplished by merging strong nanoscience and chemistry competences in surface chemistry, electrochemistry, and the "wonder material" graphene. Our research is currently housed under the new Danish National Research Center, Carbon Dioxide Activation (CADIAC).

It is now generally accepted that high atmospheric concentrations of CO<sub>2</sub> from the burning of fossil fuels pose threatening changes to our climate. Our contribution to solving this pertinent problem consists of the development of nanotechnological methods by which it becomes possible to use CO<sub>2</sub> as a valuable resource for the synthesis of fuels and platform chemicals. The innovative aspect of our work consists of deliberately arranging both CO<sub>2</sub>, captured from the atmos-



phere, and electrocatalysts in optimal three-dimensional graphene derived structures to achieve a hitherto unseen activation of CO<sub>2</sub>. In this manner materials that display outstanding catalytic activity and selectivity at the same time may be generated.

In addition to the synthesis of novel functionalized materials, we use numerous characterization techniques in our daily work, including XPS, ToF-SIMS, Raman, PM-IRRAS, and AFM.

Many of our projects have an applied focus and involve collaboration with industry partners such as Grundfos, SP Group, Kamstrup, Vestas, Newtec, and LEGO. Furthermore, our work has led to the creation of a start-up company, RadiSurf, which commercializes sealing technologies and know-how.

### FUNCTIONAL PROPERTIES OF **PLASMA PROTEINS** AND EXTRACELLULAR MATRIX

Laboratory for Proteome Analyses and Protein Characterization, Jan J. Enghild, PhD in protein chemistry, Professor

The group is interested in plasma proteins and the extracellular matrix (ECM) and its crosstalk with normal and pathological processes, in particular the regulation of proteolytic activity and the influence of post-translational modifications on protein function.

The extracellular matrix (ECM) is where all cells live; they do not just function as a mechanical support for the cells, but are dynamic structures that provide signals to regulate cell adhesion, cell-to-cell communication, differentiation and inflammation. An example from the lab of this interplay involves the bikunin proteins. These are found in the blood although they mainly play a role in the ECM. The



proteins have a unique structure where the subunits are covalently cross-linked by a glycosaminoglycan chain. This cross-link is able to participate in a transesterfication reaction where the heavy chains of the bikunin proteins are transferred to other glycosaminoglycan molecules in the ECM. This process participates in the mechanical stabilization of the ECM with impact on cell adhesion and migration. The other major research area in the laboratory is plasma proteins. Here we mainly focus on the characterization of coagulation- and fibrinolysis-related proteins. We use a combination of protein chemistry, proteomics, targeted mass spectrometry, enzymology, and recombinant DNA techniques to address scientific problems of interest.

### BIOELECTRONIC NOSES AND PSYCHOELECTRO-CHEMISTRY

Electrochemical Biosensors and Bioelectrocatalysis Group, Elena E. Ferapontova, PhD in electrochemistry, kinetics og catalysis, Associate Professor

We study and use electronic and structural properties of nucleic acids and enzymes to develop advanced nanobiotechnologies for health care, food and environmental biosensors such as bioelectronic noses and tongues, novel bio-energy and bioelectronic nanomaterials and for psychoelectrochemical research.

We develop nanotechnologies that exploit the electron transfer properties of DNA tethered to electrodes, crucial to the operation of molecular bioelectronics and electrochemical non-invasive biosensors for protein and  $\mu$ RNA cancer biomarkers, selective analysis of neurotransmitters in brain models (psychoelectrochemistry) and food spoilage screening.



In another research direction, biotechnologically challenging enzymes are chemically/genetically modified by tags or reconstituted on their cofactors conjugated to conductive linkers. Tagged proteins are in an orientated way immobilized on electrodes to obtain the most efficient electrochemically modulated electron transport through the protein and bioelectrocatalysis, which is then used in electrochemical biosensors for clinically important analytes and for sustainable energy production in hybrid biofuel cells.

Our projects, such as the current NUMEN project focused on the development of ultrasensitive biosensor nanotechnologies for analysis of pathogenic microorganisms in air and water, include industrial collaborations with several companies such as sensor-producing Unisense, pump-producing Grundfos, air-analyzer producer TSI Inc.

### NEW STRATEGIES FOR SMART BIOMATERIALS

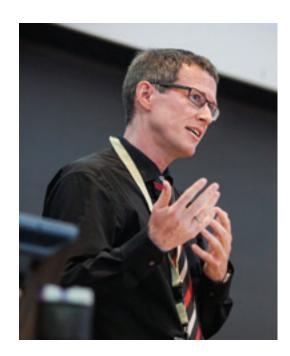
Biomedical Surface Group, Morten Foss, PhD in physics, Senior Researcher

The main objective of our research is to gain fundamental insight into the interaction between artificial and biological systems of biomedical relevance. With this knowledge, we aim to develop new strategies for smart biomaterials with a view to solving some of the major biomedical challenges society is facing today.

We study protein adsorption, mammalian cell behavior and tissue response with respect to functionalized biomaterials. In terms of specific applications, the current research focuses on the synthesis of novel micro- and nano-functionalized implant materials, large-scale screening of surface cues for guided cellular response, and non-fouling surfaces. For example, we are currently examining the influence of a tailored local release of strontium from implants on cellular response and periimplant bone healing. We are also developing new non-fouling coatings with superior properties as compared to the current state-of-the-art.

Understanding the implant-tissue interface requires a range of multidisciplinary characterization techniques spanning across physics, chemistry and molecular/cell biology.

The group has a strong collaboration with the biomedical industry and a number of national and international scientific groups. At present these projects include bone contacting implants, soft tissue/implant integration and percutaneous implants.



### TRACING MOLECULAR PROCESSES – **IN BIOFUEL FORMATION** AND THE ATMOSPHERE

Atmospheric and Analytical Chemistry Group, Marianne Glasius, PhD in chemistry, Associate Professor

We develop and apply advanced analytical methods to detect molecular tracers of chemical processes, whether these occur during hydrothermal liquefaction of biomass to develop new biofuels or are involved in the formation and growth of atmospheric aerosols.

Our research addresses some of the major issues in society today, namely air pollution, climate change and the development of alternative fuels. We use our analytical expertise to investigate chemical processes from molecular to global scales. The analyses demand a suite of instruments to detect molecules with a wide range of properties regarding volatility and polarity. We develop analyses using gas chromatography coupled to mass spectrometry (GC-MS) with specialized injection methods, and ultrahigh performance



liquid chromatography coupled to quadrupole time-of-flight mass spectrometry (UHPLC-qTOF-MS) for analysis of polar compounds to provide information on the exact chemical composition. These analytical methods are also applied to study other topics such as novel food ingredients.

Our projects are often carried out in national and international collaborations, e.g. when we study aerosols in Greenland or develop sustainable high-value ingredients and biofuels together with industrial partners. From July 2014 to July 2015 I am on a research stay at University of California, Berkeley, USA, to investigate new, innovative approaches for probing the chemical composition of complex matrices.

## **DNA NANOTECHNOLOGY**– SELF-ASSEMBLED NANO-STRUCTURES AND DEVICES

Professor Kurt Gothelf and his Centre for DNA Nanotechnology (CDNA) are exploring the application of DNA for the formation of functional nanostructures and their application in various fields such as molecular electronics, biosensors and drug-delivery vehicles.

DNA is an amazing molecule that contains the genetic information in all life forms. From a chemical point of view DNA is also completely unique since it is the only type of molecule that can be programmed to assemble into predesigned structures with high reliability. This enables the formation of structurally well-defined nanostructures formed solely by self-assembly.

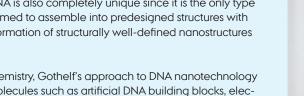
With a background in organic chemistry, Gothelf's approach to DNA nanotechnology is based on preparing organic molecules such as artificial DNA building blocks, electronically interesting molecules, e.g. conducting wires, dyes, for DNA nanotechnology and the development of new chemical methods applied to bionanotechnology.

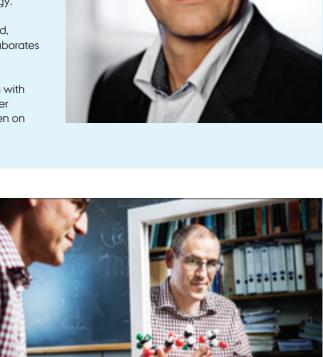
Although DNA nanotechnology is a young and mainly academic research field, Gothelf is also aiming at practical applications of the technology, and he collaborates on DNA based projects with companies such as Vipergen and Unisense.

The research at CDNA is highly international and is performed in collaboration with research groups at three American universities associated with CDNA and other researchers in Europe and China. Several students in Gothelf's group have been on research visits to Harvard, Arizona State and North Carolina State Universities.

ANY RIGHT MOLECULES

LEFT?





Theoretical Surface Science Group, Bjørk Hammer, PhD in physics, Professor

In our work we use quantum mechanical computer simulations to model the formation of chiral molecules over achiral solid surfaces. To introduce a stereo-selective driving force, the surfaces are changed through the presence of chiral "modifier" molecules that eventually lead to the formation of an uneven amount of "right" and "left" product molecules. In our work we seek to understand which elementary interaction processes are responsible for this behavior. '

We collaborate with a group at Laval University in Quebec that does scanning tunneling microscopy (STM) of highly catalytic Pt surfaces modified with trace amounts of chiral modifier molecules. Upon the introduction of reagents (various alpha-keto esters and hydrogen) the role of the modifiers appears to involve the formation of modifier-reagent pairs. These pairs have asymmetric appearances in the STM images and in the ideal case their presence implies that either only left- or right-handed product molecules are left after reaction on the surface.

Our computer simulations help reveal the atomic structure within the modifier-reagent pairs and are key to understand what type of interactions happen between the reagent, the modifier, and the surface. The simulations further uncover aspects of how the surface acts catalytically and of the nature of the different chemical and physical bonds formed.

Future work aims at using the computational approach to propose and test new modifier molecules with improved enantioselectivity.

### 29

Organic Nanochemistry Group, Center for DNA Nanotechnology, Kurt Vesterager Gothelf, PhD in inorganic chemistry, Professor

# **TO PACK OR** NOT TO PACK?

Functional Organic Materials Group, Michael Ryan Hansen, PhD in chemistry, Assistant Professor

The aim of our research is to understand how organic materials organize and behave dynamically at the molecular level, which establishes their specific function in many cases. Our scientific approach is based on a combination of experimental and theoretical techniques allowing us to address different length and time scales.

We elucidate how soft matter, ranging from small organic molecules to larger macromolecules, self-assemble into functional materials via solution or melt-state processing. This includes materials based on conventional polymers, block copolymers,  $\pi$ -conjugated polymers, gels, in addition to graphene and graphene-based nano-composites. One of our current research projects focus on the characterization of morphology and molecular interfaces in organic-based solar cells.



The elucidation of how soft matter is organized and behaves dynamically at the molecular level is, however, a challenging task, since such materials typically show pronounced semi-crystallinity. To tackle this challenge, we employ a combined experimental and theoretical approach using x-ray diffraction (XRD), solid-state nuclear magnetic resonance (NMR), and density functional theory (DFT) calculations. By combining these methods, we are able to establish a much broader picture of short- and long-range order in addition to gaining insights into dynamical processes.

Our current research projects involve collaborations with national and international academic partners. Future projects aim at setting up more applied projects in collaboration with industry.

INDIVIDUALITY MATTERS

> iDEAs Group, Megan Yi-Ping Ho, PhD in mechanical engineering, Assistant Professor

The goal of iDEAs (Innovation, Design, Engineering, Application in Single Cell) is to establish a single cell platform to study the "nanobio" interface and how cell fate is altered by environmental and therapeutic stimuli. Ultimately, the generated knowledge will lay the foundation for future diagnostics and therapeutics.

Cellular heterogeneity is intrinsic to many cell-fate processes; however, traditional biological analysis often relies on averaged phenotypic information and overlooks the heterogeneous responses among cells. In iDEAs, we focus on the study of molecular and cellular dynamics in a single cell manner. Particularly, we would like to address issues on the "nano-bio" interface, where synthetic therapeutic materials are in contact with biological components. Our strategy to



approach the cellular heterogeneity is through the development of DNA nanosensors and microfluidics. These tools will help us to access the dynamics of cells with high temporal and spatial resolutions. The merit will eventually make us able to design and modify nanomaterials with a view to tackling various biological problems and upcoming clinical challenges.

Our projects involve strong interactions between academic and industrial partners. As an example, recent progress in our research efforts has spun out as a start-up company called Zymonostics, which focuses on the development of DNA nanosensors for the detection of infectious diseases.

### **CARBON SURFACES** FOR INDUSTRY AND SPACE

Surface Dynamics Group, Liv Hornekær, PhD in physics, Associate Professor

Our research is aimed at understanding and controlling the electronic and chemical properties of carbonaceous surfaces at the atomic level and to use this understanding for the development of new materials for electronics, anti-corrosive coatings and models for interstellar chemistry.

We synthesize and study high quality graphene, a single layer of graphite, on metal surfaces and investigate how the electronic properties of the graphene can be controlled by chemical functionalization or by the intercalation of species at the graphene-metal interface. Furthermore, we investigate under which circumstances high quality, single layer graphene can be used as an anti-corrosive coating and how chemical functionalization influences coating performance. We also study the catalytic properties of carbonaceous systems with specific emphasis on interstellar chemical reactions. We use a broad range of surface science techniques to gain deep insight into the physics and chemistry of the systems we study. In particular, we use scanning tunneling microscopy to obtain atomic level information on surfaces and functionalization structures.

Many of our projects have an applied focus and involve collaboration with academic and industrial partners. These projects include: Synthesis of high-quality graphene films (DA-GATE) and development of anti-corrosive graphene coatings (NIAGRA).

### BIG IMPACT WITH SMALL THERAPEUTICS

NanoPharmaceutical Lab, Kenneth Howard, PhD in pharmaceutical science, Associate Professor

The group works on the development of advanced drug delivery technology for therapeutic intervention of diseases with a focus on understanding biological barriers required for optimal design of nanoscale carriers.

We work on polymer-based therapeutics and surface engineering of nanoparticles with stealth and targeting "nanoshells" and the application of advanced surface characterisation techniques, such as X-ray photon electron spectroscopy (XPS), to determine amount and arrangement on the outmost 10 nm surface that is a predominant factor in determining biological interactions. As an alternative, we are harnessing the natural role of albumins to act as a transport protein for drug delivery applications. Biological effects are evaluated in a number of cell types and animal models using flow cytometry, confocal microscopy and live animal imaging. Understanding and exploiting transport across mucosal surfaces is being used as treatment strategy for inflammatory bowel disease (IBD) by designing nanocarriers that disassemble on interaction with the mucus barrier to release anti-inflammatory nucleic acid therapeutics. A focus of the lab is the application of RNA interference therapeutics against molecular targets evaluated in disease models for rheumatoid arthritis and IBD. The lab has extensive collaboration with national and international industrial partners on projects ranging from the design of RNAi therapeutics to controlling receptor-mediated transport of nanocarriers.





### FROM ATOMIC STRUCTURE TO APPLICATION



Center for Materials Crystallography, Bo Brummerstedt Iversen, PhD in inorganic chemistry, Professor

Crystalline materials form the core of numerous modern technologies, and detailed understanding of the crystal structure is the basis for rationalizing and improving any useful properties the material may possess. The Center for Materials Crystallography (CMC) has outstanding facilities to synthesize materials, and a broad range of X-ray and neutron scattering techniques are used to investigate their structures. Simultaneously, we quantify properties using a wide range of techniques.

Our studies range from fundamental research to applied science. A few examples related to energy technology include i) thermoelectric materials that can harvest electricity from waste heat, ii) Alkali ion batteries both for high power density and large-scale storage, iii) nanocatalysts for fuel cell applications, and iv) nanocrystalline photocatalytic materials for use in, e.g. solar cells. CMC has a very active program on chemical synthesis using supercritical fluids as well as a strong focus on the development of novel crystallographic tools. This includes in situ reactors for the study of nanocrystal formation and growth, or techniques for experimentally measuring electron densities in crystals.

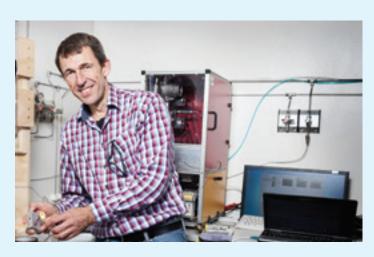
CMC is involved in many collaborative projects with industrial partners such as TEGnology (thermoelectrics), Haldor Topsøe (battery materials), Widex (fuel cells), Dinex (catalysts) and the Danish Technological Institute (supercritical synthesis).

### **STORAGE OF RENEWABLE ENERGY** – A CLEAN FUTURE

Inorganic Nanomaterials Group, Torben R. Jensen, PhD in materials chemistry and dr.scient., Associate Professor

The aim of our research is to prepare new materials with interesting structures and properties and to develop new synthesis and characterization methods. The fundamental science knowledge is utilized for rational design of novel materials for energy storage in hydrogen or in batteries, porous materials for nanoconfinement, gas separation and selectivity, or conversion of carbon dioxide into useful fuels.

The ambition is to conduct cutting-edge international research on new inorganic 'energy materials' and chemical reactions relevant to important technologies and to develop new concepts for energy storage, e.g. hydrogen storage in light element solids, nanoconfinement of metal nanoparticles, hydrides or composites, conversion of  $CO_2$ back to useful fuels and battery materials. Novel combined mech-



ano-chemical and solvent based methods are of key importance along with synchrotron powder diffraction. The group also develops new equipment and approaches for thermal analysis and thermodynamic and kinetic characterization of gas release and uptake.

The group is in charge of the largest Danish 'hydrogen' project HyFill-Fast funded by the Danish Council for Strategic Research (total budget of DKK 39 million) and has a leading role in four EU funded research initiatives, which include many industrial companies. In addition, the group leader acts as an expert for the international energy agency. The very dynamic and productive group consists of about 20 people and has published 105 peer reviewed journal papers since 2010, and these new publications have already been cited 1350 times.

### **PROTEASES IN HOMEOSTASIS** AND DISEASE

Proteases are enzymes which catalyse the hydrolysis of peptide bonds. Humans have 569 different proteases. Some proteases have aggressive and non-specific protein-degrading abilities and function in the digestive system. Other proteases are highly specific and catalyse the hydrolysis of only a specific peptide bond in a specific protein, for instance a specific peptide bond in an inactive precursor of another protease, which is thereby activated. In this way, proteases can be arranged in cascades, in which one protease activates the next one in the line. Such cascades are found in blood coagulation, regulation of blood pressure, and defense against microorganisms.

The normal functions of proteases rely on strict regulatory mechanisms, ensuring controlled and localised activation and finally inhibition by specific and fast acting protein protease inhibitors. When regulation does not work properly, disease will occur. The abnormal function of proteases is involved in the pathogenesis of diseases spanning infectious diseases, thrombosis, and cancer.

Our group is particularly interested in the protease systems involved in the modeling and remodeling of tissues, such as the development of skin and wound healing. We are interested in finding compounds that can correct abnormal protease function and thus alleviate diseases. Our research is interdisciplinary as we combine molecular biological technologies with biophysical techniques. We elucidate the molecular details of specific protease systems. We isolate protease inhibitors or stimulators from combinatorial libraries and characterize their interaction with the proteases. To do this, we use X-ray crystal structure analysis, NMR, SAXS, ITC, SPR, *i.e.*, a broad spectrum of techniques available at the iNANO Center. Our research is international and funded by grants to a variety of international collaborative projects. Associate Professor, PhD in nanotechnology, Jan K. Jensen Postdoc, PhD in nanotechnology, Daniel M. Dupont



Professor, dr. scient. Peter A. Andreasen



### SQUEEZING LIGHT OUT OF SILICON

Semiconductor Group, Brian Julsgaard, PhD in physics, Associate Professor

Silicon is one of the most important elements in modern technologies as it forms the backbone of nearly all electronic components from individual transistors to large computer processors. However, one serious drawback of silicon is its unwillingness to emit light.

One possible way to squeeze light out of silicon is to embed into it another material which does emit light. In our research we embed nanostructures of other group-IV elements, and we are particularly interested in tin, which in principle is an efficient light emitter. Optical characterization of the nanostructures is mostly undertaken by time-resolved fluorescence measurements, which enable us to "see" the separate physical processes behind the light emission.



The nanostructures are formed by molecular beam epitaxy (MBE), i.e. grown layer-by-layer on the atomic scale with a low concentration of defects and dislocations. To examine the quality and geometry of the nanostructures, we use many techniques including high-resolution transmission electron microscopy (TEM).

Efficient light emission inside silicon would allow for a true integration of electronic and optical functionality on a single chip and thereby increase the speed of computers and their interconnection.

### **BROAD AS A LAMP** AND BRIGHT AS A LASER

Femtolab, Søren Rud Keiding, Dr.scient., Professor

Light is the primary tool we use when "talking" to atoms and molecules, and the development of new light sources and spectroscopic techniques is a key research theme in the Femtolab. The goal is to make light sources "broad as a lamp and bright as a laser". This is done using very short (femtosecond) optical pulses in combination with optical fibers. The sources are called super continuum sources (SuperK). Together with the Danish companies FOSS and NKT we are using these new SuperK light sources in food, water, and soil analysis. We are also employing femtosecond laser pulses to study the dynamics properties of liquid water, in particular its ability hold to exchange energy and shield charges during chemical reactions.



Finally, we are using lasers to hold and manipulate small micro(nano) scopic particles in an optical tweezer.

Our contributions are directed towards the development of new lasers and spectroscopic techniques. The challenge is to investigate the molecular mechanisms behind the observations. We spend approximately 50% of our time developing new experimental techniques and the rest on specific molecular systems under investigation.

### INTERFACING NANOSTRUCTURES WITH CELLS

Nucleic Acid Technology Group, Jørgen Kjems, PhD in chemistry, Professor, Director of iNANO

Our main interest is to design artificial nanostructures that can interact with cells and whole organisms and enable sensing, diagnosis and therapy of human diseases.

Using disease specific markers as guides, we are developing new targeted nanoparticles to carry nucleic acid based drugs to diseased cells for gene targeting. In a related line of research the particles are equipped with fluorescent or superparamagnetic material to allow bioimaging of pathological conditions. To create modular and flexible carrier system for combined biosensing, drug delivery and bioimaging, we are exploring the capacity of RNA and DNA to form self-assembled 3D structures, functionalized with complex patterns of proteins, sugars and lipids.



We are also developing systems for improved gene knock down based chemically improved small interfering RNA (siRNA), microRNA and, as a new principle, circular RNA molecules (circRNAs) and applying them to relevant disease models including Parkinson's disease, epilepsy, viral infections, inflammation and cancer. We are also integrating gene specific drugs with 3D printed biodegradable scaffold to spatially control the differentiation of stem cell into specific cell types with the intention, one day, to rebuild tissue and even organs in humans suffering from regenerative diseases.

### MOVING TARGETS: CAPTURING MOLECULES IN 3D

Visualization Lab, Rikke Schmidt Kjærgaard, PhD in science communication, Associate Professor

The main goal of the Visualization Lab is to produce a new graphic standard framework for molecular and nanoscale science. We develop exploratory 3D animations specific for bio-nanoscience data analysis using high-end 3D software.

The Visualization Lab develops innovative visual solutions for contemporary scientific imagery, creates integrated visual systems based on graphic design and animation, and advances educational strategies in science visualization for scientists. We teach visualization methods and design principles to PhD students and postdocs from the sciences.

By studying graphics, art and design principles and connecting them to scientific data analysis, we explore new ways of visually commu-



nicating data, and investigate if and how these new visuals help scientific analysis. We are currently exploring new ways of visualizing bacteria and their cellular and molecular data by using unconventional methods such as watercolour and animation.

Currently, we have an artist-in-residence making an installation by combining nanotechnology and art. We hope to continue this artist-in-residence programme in the future. The Visualization Lab connects researchers all over the university with an interest or goal in data visualization. In a monthly interdisciplinary journal club gathering researchers from the sciences and humanities, we discuss our projects and scientific data from a visual point of view.

### WATCHING SINGLE PROTEINS DANCE

Protein Dynamics Magnus Kjærgaard, PhD in biochemistry, Scientific Researcher

Our overall goal is to understand the molecular mechanisms underpinning the function of the nervous system. We focus particularly on studying the internal movements of membrane proteins using single molecule fluorescence microscopy, and how these movements affect the interactions with other proteins.

Biological cells use membrane proteins to exchange information and material with their surroundings. Intramolecular movements are crucial to the function of these proteins as signals are often transmitted as a structural change and the transport of molecules often requires interconversion between different states. Traditionally, it has been difficult to observe the dynamics of membrane proteins. However, recent developments in ultra-sensitive light microscopy have enabled the observation of light emitted from single molecules, paving the way for studies of the movements of single membrane proteins. We use these single molecule fluorescence techniques to study the dynamics of part of membrane pumps and ion channels; proteins that are crucial to the communication between nerve cells.

We use these approaches to understand how mutations can lead to neurological diseases and how memories are stored in the physical structure of the brain. We are affiliated with the recently established DANDRITE neuroscience center, which spans a wide range of topics within neuroscience.

**ENZYME ACTIVITIES** AS TARGETS FOR DIAGNOSIS AND PREDICTION OF TREATMENT RESPONSE

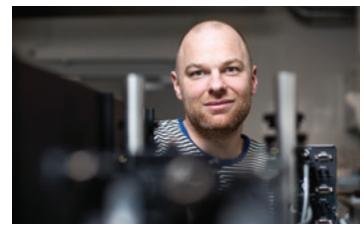
> DNA Biosensor Group, Birgitta Ruth Knudsen, PhD in molecular biology, Associate Professor

The goal of our research is to elucidate the functions of life-essential enzymes from humans or pathogens targeting humans and use this knowledge to generate biosensors for the detection of human diseases such as malaria or tuberculosis, or for the prediction of the outcome of cancer treatment.

We study the molecular mechanisms of DNA-interacting enzymes to elucidate the specific features that allow for the development of specific DNA-based biosensors to detect their activities. Most of these biosensors are adapted for optical detection using fluorescence or direct visual color reactions, but future work will also focus on electrochemical read-out methods. In our work we combine molecular biology with nanoscience to develop innovative methods for hypersensitive monitoring of enzyme activities at the single-molecule or single-cell levels. Such methods can be used for the diagnosis of, e.g. malaria, and they are used to investigate some of the important factors behind chemoresistance in anti-cancer treatment. In the future we hope to contribute significantly to personalized cancer treatment.

Many of our projects have an applied focus, and some of our research has resulted in the start-up of the spin-out company Zymonostics, focusing on developing rapid, sensitive and specific methods for the diagnosis of infectious diseases.





# **CATALYSTS** UNDER THE MICROSCOPE



Nanocatalysis Group, Jeppe Vang Lauritsen, PhD in physics, Associate Professor

Our research provides atomic-level insight into the working principles of catalytic nanomaterials. The aim is to rationally design catalysts on this fundamental knowledge base for use in better environmental protection technologies and renewable energy production.

We investigate how we can control nanoscale properties such as nanoparticle size, shape and surface structure to improve catalytic activity. We carry out this research by imaging catalyst surfaces under the influence of reactants directly at the atomic scale by using a range of scanning tunneling microscopes (STM) and atomic force microscopes (AFM). A current research goal is to develop improved catalysts for the reduction of smog problems caused by NOx and SOx emissions. A key to catalyst development is to understand how support materials can be chemically modified or nanostructured to better anchor the nanoparticles in a bottom-up process. This research theme is pursued for the Cu/ZnO catalyst used for methanol synthesis (a possible biofuel) and various metal catalysts on the most common support in industrial catalysts, Al<sub>2</sub>O<sub>3</sub>.

Although our research on catalysis is fundamental in character, it is of distinct importance to the catalysis industries, and we collaborate with several companies and research institutes. Catalysis is a truly interdisciplinary research area and we continuously look for new opportunities for collaborations.

# SEEING **MOLECULES** AT PLAY

Molecular interactions on surfaces and the formation of molecular surface nanostructures are central to many application areas within nanotechnology and also constitute idealized model systems for many important processes in nature. We strive to obtain detailed microscopic insights into the fundamental principles underlying molecular self-assembly, reactions and dynamics on surfaces and apply these towards the synthesis of new types of structures.

Our research is based on an ultra-high vacuum surface science platform employing high-resolution variable temperature scanning tunneling microscopy (STM) as the main technique. We use this platform to study supra-molecular self-assembly on surfaces, including bio-molecular adsorption and surface chirality. Dynamic surface processes such as molecular diffusion and conformational changes are visualized at the sub-molecular level by fast-scanning STM movies. A key focus is to develop advanced and robust surface functionalization, e.g. in the form of 2D metal-organic coordination networks or covalently interlinked molecular nanostructures formed by on-surface synthesis.

Our work often involves collaboration with groups within organic synthesis and theoretical modeling, both at iNANO and internationally. We have formed part of several European Ph.D. training networks and integrated projects.



Surface Self-Assembly and Reactions Group, Trolle René Linderoth, PhD in physics, Associate Professor

### BRIGHT HYBRIDS



Hybrid Materials Group, Nina Lock, PhD in chemistry, Assistant Professor

The overall aim is the development of new porous hybrid organicinorganic materials for heterogeneous- and photocatalysis as well as optical applications. The functionality of the compounds can be tailored by combining the properties of the organic and inorganic constituents with the porosity of the resulting 2D and 3D materials.

Organic-inorganic hybrids are sophisticated materials composed of organic as well as inorganic structural motifs, and they uniquely adopt properties of both components. Hybrids count several classes of compounds including: a) 3D metal-organic frameworks (MOFs) in which metal centers are connected via organic linkers, and b) 2D inorganic layers with metal-organic complexes sandwiched inbetween. My current research focuses on the development of novel layered semiconducting tin sulfides functionalized by metal-organic complexes or organic dyes. The aim is to understand the influence of these light absorbing molecules on the absorption-, emission- and photocatalytic properties of the hybrid materials. Another material class in focus is 3D MOFs, which are functionalized with transition metal complexes for heterogeneous catalysis. The ultimate goal of this research is the activation of small molecules such as water and  $CO_{\gamma}$ .

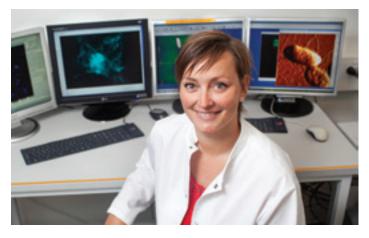
I am affiliated with the Danish National Research Center CADIAC at Aarhus University, which focuses on  $CO_2$  activation. The center has just been established, and new projects will focus on the development of hybrid materials for  $CO_2$  capture and conversion.

### THE COMBAT AGAINST **BIOFILM**

Biofilm Group, Rikke Louise Meyer, PhD in microbiology, Associate Professor

The overarching goal of our research is to achieve a fundamental understanding of the biological mechanisms involved in bacterial biofilm formation, and to use this knowledge to combat biofilms, either by preventing their formation or by developing more effective treatment strategies.

We study the mechanism of bacterial adhesion by identifying and investigating the functionality of key biomolecule adhesins that allow bacteria to attach to abiotic surfaces and to other cells. We are currently investigating the role of extracellular DNA in adhesion and biofilm formation by *Staphylococcus* species, and we are discovering new genes that regulate biofilm formation in *Bacillus cereus*. We combine molecular microbiology with a range of biophysical methods to characterize the cell surface properties and visualize



biofilms by confocal laser scanning microscopy (CLSM) and atomic force microscopy (AFM).

Understanding the interaction forces of bacterial cells is a core issue, and we use our AFM to do single-cell force spectroscopy. These measurements quantify the adhesion force of the cell to other cells or to different types of abiotic surfaces.

Many of our projects have an applied focus and involve collaboration with academic and industry partners. These projects include: Development of antifouling surfaces for the water sector, development of treatments for biofilm infections, and formulation of natural antimicrobials for food preservation.

### FUNCTION AND FLEXIBILITY OF PROTEIN MOLECULES

Biological NMR Spectroscopy, Frans A. A. Mulder, PhD in chemistry, Associate Professor

Proteins are Nature's workhorses. They literally decide the life and death of our cells. In our group we are interested in the molecular understanding of protein biochemistry, and we use NMR spectroscopy and the proven concepts of quantum and physical chemistry to do so.

Nuclear magnetic resonance (NMR) spectroscopy is a technique that studies the atomic nuclei in molecules. NMR can reach deep down to the molecular level and make us able to study molecules at the sub-nanometer (< 0.000001 mm) scale. NMR is a routine molecular fingerprinting technique in chemistry, and is increasingly being used in food and medical sciences to characterize and quantify complex mixtures of molecules in for example milk, wine, tea, blood and urine.



At iNANO we use NMR spectroscopy to determine the structures of proteins in their physiological, watery milieu, since 3D structures provide important insights into protein function. We also go one step further, and map out their flexibility, dynamics and electrostatic behavior. The integrative understanding of these fundamental biomolecular properties is essential to achieve a comprehensive understanding of biological processes at the nanoscale.

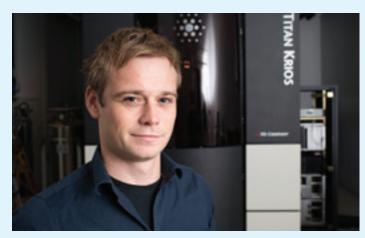
Our projects focus on the innovation and development of novel techniques and approaches, and we are involved in numerous collaborations with international academic and industrial partners about the application of NMR, ranging from the improvement of barley seed quality to the molecular basis of Alzheimer's disease.

A DIRECT VIEW ON MACROMOLECULAR MACHINES

> BioTEMLab, Arne Möller, PhD in biology, Assistant Professor

My group uses 3D Electron Cryo Microscopy (cryo-EM) to determine the structure of macromolecular machines. Cryo-EM can be referred to as "bridge to the cell", as it is uniquely suited to image a large array of protein complexes in a quasi-native environment. EM is a direct imaging method that literally allows us to "see" the proteins under investigation.

My lab focuses on 3D structures of dynamic protein complexes. Using cryo-EM, we are currently investigating the essential ATPase p97 involved in numerous cellular functions and Sortilins, membrane protein receptors that are key players in many neurological disorders. Both interact with a large array of binding partners, which specifically alter the function of the protein. We want to determine their 3D structures



to characterize the modes of binding. This information is crucial to fully understand the mode of action and to develop strategies for the development of site-specific therapeutics.

The lab is also actively pursing method development, including new software tools and optimization of sample preparation. In collaboration with the group of Assistant Prof. Ebbe Sloth Andersen we have started to utilize specifically engineered RNA origamis as markers for proteins that would otherwise not be detectable by cryo-EM.

At the iNANO Center we have now established a state-of-the-art cryo-EM facility, which will also be accessible to scientists outside AU, and which targets a plethora of interesting biological questions.

# **UNDERSTANDING WATER TRANSPORT** AT THE PLASMA MEMBRANE LEVEL

Group of Lene Niemann Nejsum, PhD in cell biology, Associate Professor

Aquaporin water channels facilitate transepithelial water transport and are key in regulating body water homeostasis. Our aim is to understand how aquaporins are regulated in the plasma membrane with the long-term aim of potentially modulating plasma membrane levels, and thus, targeting body water balance disorders.



We specifically study how aquaporins responsible for urine concentration diffuse, interact and how they are organized in the plasma membrane at the nanoscale. We use a combination of cell biology, live-cell imaging, super resolution microscopy, protein patterning and biophysical methods to investigate how aquaporins are regulated in different membranes of the cell in response to physiological stimuli.

# MEMBRANE PROTEINS

IN NEUROSCIENCE AND DRUG DISCOVERY

DANDRITE, Poul Nissen, PhD in molecular biology, Professor of protein biochemistry

We study the atomic structure, mechanism and cellular function of membrane transport proteins. Our biological focus is on neuroscience with key questions on how membrane transport proteins orchestrate neuronal signaling networks in the brain and how these are affected in neurological and psychiatric diseases.

More than half of the energy consumed in the brain is used by P-type ATPase ion pumps that maintain electrochemical gradients for, e.g. Na<sup>+</sup>, K<sup>+</sup> and Ca<sup>2+</sup>. These gradients energize numerous other processes in cell membranes such as neurotransmitter transporters, ion channel receptors, and Ca<sup>2+</sup> signaling pathways. Similarly, P4-ATPase lipid flippases maintain the asymmetric distributions of lipids in the biological



membranes as required for, e.g. vesicle-mediated signal transmission, cellular trafficking, and lipid-based signaling.

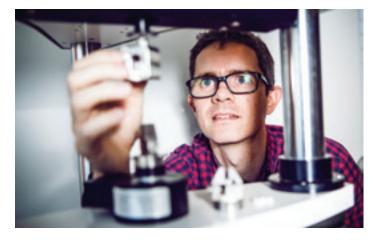
We study the structure and function of these membrane transporters and how they relates to key functions in the brain. A long-term goal is to understand the higher-order structure of brain cell membranes. We use primarily membrane protein crystallography, biochemistry, electrophysiology, and fluorescence spectroscopy. Furthermore, we are implementing new approaches in cryo-EM and EM tomography. Our research provides "first views" of new opportunities in drug discovery and biotechnology, so we are also pursuing spin-out and start-up activities and industry collaborations.

# **DIGITAL MATERIALS** ENGINEERING

Mechanical and Materials Engineering Section at the Department of Engineering Jens Vinge Nygaard, PhD in mechanical engineering, Associate Professor

Mechanical engineering is about studying the fundamental mechanisms behind any movement and the energy converted in the process of moving. Materials engineering is about applying the properties of matter to engineer devices exploiting internal structures within the materials, and thereby dictate how the material moves or redistributes energy internally once in service.

Engineering is also about making new technologies, and access to advanced materials has often driven technological breakthroughs. The usage of composite materials enables us to engineer enhanced performance, or build additional function into the material. Access to well-characterised polymers, improved control, and enhanced automation in materials processing have led to the development of materials printing – 3D printers. Coupled with nanotechnology, new



ways emerge to build and assemble advanced material structures into 3D composites at shorter length scales. Mechanical engineers use computer aided design tools to synthesize the geometry of any product and mathematically investigate its performance, and the tools are applicable to nanofabrication. Thus, materials engineering is becoming a digital development cycle.

Our current projects focus on the synthesis of bioactive medical devices manufactured by additive techniques such as fused deposition modelling and electrospinning. They are used for tissue engineering of connective tissue in the pelvic floor region and cartilage in the joints of the skeletal system. The projects are carried out in collaboration with Aarhus University Hospital and Biotech Companies.

**PROTEIN AGGREGATION:** THE DARK SIDE OF THE FORCE

> Protein Biophysics Group, Daniel Otzen, PhD in protein biophysics, Professor

We aim to understand in molecular detail how protein aggregates are formed in sickness and in health. This knowledge is used to combat neurodegenerative diseases and other misfolding disorders as well as to develop self-assembling material.

We study how proteins associate to form long fibrils (amyloid) as well as smaller oligomers. We focus on  $\alpha$ -synuclein (involved in Parkinson's disease), proteins in corneal dystrophy, other amyloid-forming disease-associated proteins and also functional amyloid formed by *Pseudomonas* bacteria. We investigate by spectroscopy, light-scattering and calorimetry how aggregation can be controlled and inhibited by small molecules and surface-active compounds. We have



extensive collaborations with experts in small-angle X-ray scattering, mass spectrometry and cellular aspects of fibrillation. Thus we build up a very detailed view of the many steps involved in aggregation as well as their physiological consequences, and of how functional amyloid is formed in a very tightly controlled process. Protein self-assembly can also be promoted by free fatty acids, forming protein-lipid complexes called liprotides, which can potentially store and transport hydrophobic drugs and nutraceuticals.

We collaborate with industry and academia to develop approaches to target the cytotoxic and generally deleterious consequences of protein aggregation.

# **STRUCTURAL ORGANIZA-TION AND SELF-ASSEMBLY** ON THE NANOMETER LENGTH SCALE

Soft Matter Group, Jan Skov Pedersen, PhD in physics and dr.scient., Professor

The central topic of our research is to determine how molecules interact and self-assemble into higher order structures and provide an understanding of the mechanisms that lie behind. The knowledge is used for directing self-assembly in many types of systems and designing systems with controlled response that can be used, for example, in drug delivery systems.

Self-assembly of molecules in solution is a fundamental process in living systems as well as in many commercial products. Many types of interactions (hydrophobic, electrostatic, hydrogen bonding ...) can lead to self-assembly and the control and understanding of these interactions are crucial for the formation of stable particles and



structures. Among the systems we investigate are block copolymer coacervate micelle, lipid-protein complexes, and microemulsions. These are all systems that have applications in controlled drug delivery and which may be designed to have responsive behavior, so that release can be triggered by, e.g. temperature, ionic strength or pH changes. The experimental investigations are mainly done on the in-house SAXS equipment, and they are supplemented by a suite of other techniques.

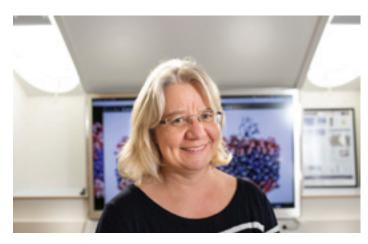
A new powerful SAXS equipment was installed ultimo 2014. It has specially designed optics and use a high intensity liquid metal jet X-ray source, and allows us to perform time-resolved measurements with a time resolution of a second.

**COMPUTATIONAL** MICROSCOPY

> Biomodelling Group, Birgit Schiøtt, PhD in chemistry, Professor

The aim of our work is to achieve fundamental insight into complex bio- and medicinal chemistry systems with atomic details. Such knowledge is invaluable for understanding fundamental properties of life, such as cell signaling and cell-cell communication, but also for developing new drugs and as a tool to comprehend the results of advanced biophysical experiments.

We study the conformational properties of proteins and other bio-macromolecules, using a broad range of computational methods. Protein-protein, protein-ligand, lipid-protein, and drug-protein interactions are all biomolecular recognition events where dynamic properties play a pivotal role. Experimentally, it is extremely challenging to obtain such insight, and simulations can thus provide the



dynamical "missing link" between structure and function. Specifically, we study how substrate and drugs bind to the monoamine transporters involved in controlling human well-being (mood, appetite, etc.), and we perform simulations to clarify the origin of cytotoxicity in amyloid diseases such as Alzheimer's and type 2 diabetes mellitus. We are also involved in studies of the function of antimicrobial peptides and G-quadruplexes that may play an important role in, e.g. cancer.

Our most important tools are supercomputers, 3D-vizualisation and advanced scripting. We collaborate with many experimental groups in obtaining this much wanted insight into the mechanisms of complex biochemical systems.

# FROM ORDER TO DISORDER

Solid-State NMR Spectroscopy Group, Jørgen Skibsted, PhD in chemistry, Associate Professor

A principal goal of our research is to explore structure and reactivity of cementitious materials, mainly by solid-state NMR techniques, and to utilize this information in the development of the next generation of sustainable cement-based materials. The reactivity can often be significantly increased by introducing structural disorder in the materials.

Our research focuses on the application of solid-state NMR spectroscopy in inorganic materials research. The main areas are cement-based materials, heterogeneous catalysts, inorganic framework structures, glasses, and new materials for hydrogen storage. Our principal field is cement-based materials. In this field academia and industry face the global challenge of developing a more sustainable cement production, since today's production is responsible for roughly



5% of the total anthropogenic  $CO_2$  emissions. We contribute to this task by the development of new cement binders based on alkaliactivated systems and new supplementary cementitious materials (SCMs) which can partly replace the  $CO_2$ -intensive Portland clinkers in cement blends. A main advantage of solid-state NMR is the equal detection of crystalline and amorphous materials. This is utilized to study disorder in the SCMs introduced either by guest-ion incorporation or thermal treatment procedures.

Our current research in both cementitious materials and heterogeneous catalysts involve collaborations with national and international industrial and academic partners.

### **APPLYING CATALYSIS** TO SOLVING MODERN PROBLEMS

Organic Synthesis Group, Troels Skrydstrup, PhD in organic chemistry and dr.scient., Professor

The principle goal of our research is to develop fundamentally new catalytic transformations and technology for the construction of important organic compounds with small gaseous building blocks.

We study catalysis based on transition metals and main group elements for promoting efficient carbon-carbon and carbon-heteroatom bond formation with low molecular weight molecules such as carbon monoxide, ethylene, hydrogen cyanide and acetylene. These small building blocks are ideal for the construction of many bioactive molecules, which are of high interest to the pharmaceutical and agrochemical industry, but also for the introduction of isotope labeling with carbon-11, -13 and -14. An additional goal is to identify



fundamentally new chemistry for the activation of  $CO_2$ , thereby providing sustainable solutions for the exploitation of this unwanted combustion product as a valuable reagent to high-value chemicals of industrial importance. This latter research is currently housed under the new Danish National Research Center, the Carbon Dioxide Activation Center (CADIAC).

Many of our projects have an applied focus and involve collaboration with academic and industry partners. Furthermore, our work has led to the creation of a start-up company, SyTracks, which commercializes carbonylation technologies and know-how.

# **CELL MIMICRY** TO ADDRESS BIOMEDICAL CHALLENGES

Laboratory for Cell Mimicry Brigitte Städler, PhD in materials science, Associate Professor

Our research aims at developing and characterizing nature-inspired approaches which can be employed to address biomedical challenges. One of those approaches is therapeutic cell mimicry.

We are developing and characterizing artificial red blood cells equipped with drug deposits for the sustained treatment of chronic diseases. The development of appropriate nanosized drug deposits, and the consideration of shear stress as an important dynamic parameter present in living organisms when biologically evaluating our drug carriers are two key aspects under investigation.

Capsosomes, carrier capsules with entrapped liposomes, are considered for use in oral enzyme replacement therapy. Important aspects in this respect are the prevention of cell internalization and preserved bio-catalytic activity of the microreactors in the intestine.



In 2014 our research interest started to move into two new directions: Artificial motility with the aim to assemble self-propelled Janus swimmers for drug-delivery applications is one of them. Additionally, we are currently assembling and characterizing bionic tissue. Specifically, our goal is to understand whether artificial cells co-cultured with biological cells have the ability to improve the health of the entire cell sheet.

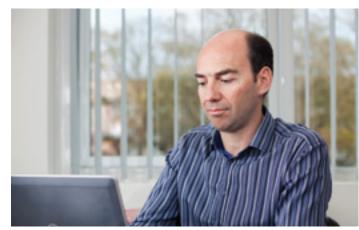
Our future research will aim at the assembly and characterization of systems not only active in biological settings, but actually addressing specific medical conditions with the prospect of being tested in vivo.

# **USING NANOSCALE ENGINEERING** TO STUDY BIOLOGICAL SYSTEMS

Nanobiointerfaces Group, Duncan Sutherland, PhD in physics, Associate Professor

We develop tools, devices and interfaces functioning at the nanoscale and apply these both to understand events in biological systems at the molecular level as well as give insight into novel materials for sensor and materials performance in biological environments.

The research in the group develops and applies nanostructured materials and sensors at interfaces and dispersed in solution as a route to quantitatively study questions in life science (e.g. protein nanopatterns to study cellular adhesion and mechanotransduction at the nanoscale, dynamic protein coronas in nanoparticle toxicity) or materials physics (e.g. plasmonic coupling in and between metallic nanostructures, thermal transfer active materials). The engineering routes and insight into interfacial interactions gained allow us to



develop new concepts in sensors (conformationally active biosensors and ultrasensitive bio/chemical sensors based on plasmonics) and surfaces (cell/ protein activating/deactivating materials and nanoparticles). The main expertise lies in integrating and applying multiple characterization tools at nanoscale interfaces to answer well-posed scientific questions and provide technical solutions within fields where biointerfaces are critical.

Innovation-directed projects focus on the development of functional materials (biomaterials, optically active materials, heat transfer materials) and sensors (bio and chemical sensors for medical and food application areas).

## **UNDERSTANDING THE "INNER ARMY"** AT THE NANOMETER LEVEL

Biophysical Immunology Laboratory, Thomas Vorup-Jensen, PhD in medicine and DMSc in nanomedicine, Professor

Several new clinical therapies target the immune system to reduce unwanted inflammation. We aim at translating the chemistry and physics of large biomolecules studied by means of nanoscience into clinical utility.

The immune system comprises several cellular and molecular components involved in defending the body against infections and cancer. When acting as a protecting "inner army", these mechanisms are of considerable benefit. It is now clear that the immune system is also capable of provoking diseases such as multiple sclerosis, arthritis, and diabetes. Molecules engaged in functions of the immune system



are often rather large, reaching 40-50 nm. Nanoscience enables descriptions of how these large molecules perform their duties in the line of defending the body or cause havoc when the immune system rebels against appropriate control. Ultimately, this insight is helpful to understand disease mechanisms and develop new strategies for treating diseases. The Biophysical Immunology Laboratory, led by Prof. Thomas Vorup-Jensen and Laboratory Manager Bettina W. Grumsen, works to understand the immune system in the perspective of protein ultrastructure and the nanoscience of the immune system.

We work to define the clinical utility of our research in a translational effort to make our research attractive for pharmaceutical development.

# UNDERSTANDING PROTEIN-LIPID INTERACTIONS

Danish Center for Ultrahigh-Field NMR Spectroscopy, Thomas Vosegaard, PhD in solid-state NMR spectroscopy, Professor

We use nuclear magnetic resonance (NMR) to study the structure and dynamics of membrane proteins and fibrillating proteins and their interaction with the cell membrane to better understand the molecular machineries and their important functions in diseases and cure.

We are constantly pushing the limits for the capabilities of current solid-state NMR methodologies to obtain new knowledge about the structure, dynamics, and protein-lipid interactions of complex molecular assemblies such as membrane proteins in the cell membrane. Our methodology-developments target the low sensitivity generally associated with NMR experiments and the level of detail obtained about the molecules in such experiments.



With the establishment of a national center in 2014 hosting the largest NMR magnet in Northern Europe and other state-of-the-art equipment, we have a strong commitment to provide an attractive platform for welcoming external academic and industrial partners within diverse fields from molecular biology to materials science. As part of this, we have established close connections with numerous academic research groups, industrial partners, and other centers in all of the Nordic and Baltic countries.

# LET THE SUN DO THE WORK!

Photocat Group, Stefan Wendt, PhD in surface science, Senior Researcher

The overarching goal of our research is to achieve a fundamental understanding of the processes occurring during (photo-)catalytic reactions on model catalysts. This knowledge may help to develop better photocatalysts for improved energy and fuel production.

We study the interaction of molecules with oxide surfaces such as titanium dioxide and iron oxide under well-controlled conditions by means of scanning tunneling microscopy (STM), temperature-programmed desorption (TPD) and photoelectron spectroscopy (PES). In such surface science experiments we use simplified model catalysts, either oxide single crystals or oxide thin films grown on a metal substrate. The high resolution of the STM technique combined with the sample-averaging spectroscopies allows us to identify the active sites of catalytic and photocatalytic reactions. Ideally, in-situ imaging of the reactions will offer a dynamic view of the behavior of reactants

on an atomic-molecular level.

An understanding of the active sites of catalytic and photocatalytic reactions is key for material design and modifications that will lead to better (photo-)catalysts. Without such research, trial-and error methods would dominate the field and an understanding of what makes a good catalyst would be lacking.

Future research initiatives include the study of the water- $TiO_2$  (anatase) interface as well as the ethanol- $TiO_2$  interface both in the dark and under the influence of ultraviolet light.

# WE THINK YOU NEED **POLYMERS!**

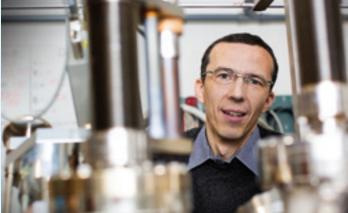
Medicinal Polymer Chemistry Lab, Alexander N. Zelikin, PhD in polymer chemistry Associate Professor

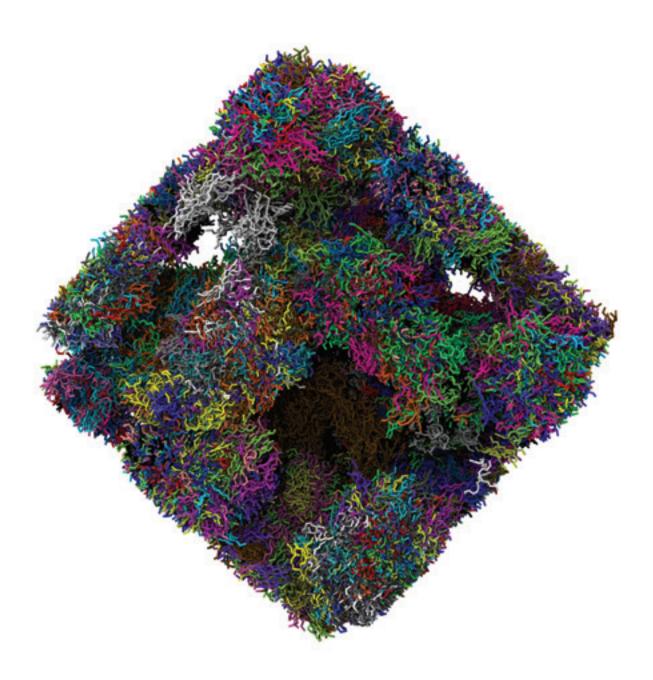
We use and further develop advanced tools of polymer chemistry and apply these to address the current challenges of biomedicine. Put simply, we are doing our best to deliver drugs in a smarter way to where it hurts.

One arm of our research considers antiviral therapy. Viruses are amazing: despite global efforts, viruses continue to be a huge socio-economic burden and a significant health care challenge. Polymers present unique opportunities to directly neutralize viruses and - oftentimes - to counter the activity of the viruses, i.e. fight viral diseases. Our excellence in chemistry is matched by the highest level of expertise in virology possessed by our partners at the Aarhus University Hospital as well as our international collaborators. We are also developing a unique approach to site-specific drug delivery using implantable biomaterials – we synthesize the drugs within the therapeutic implants. You need the drug you want, where and when you need it, and in the dose you need. OK – we are doing our best to make it happen! This research is every bit translational – that is to say, we talk to the medical and veterinary scientists as often as we can to make sure we develop what is really needed in the clinic.

Our research is highly interdisciplinary; members of our team come from different schools and departments. We are always open to new expertise so come join us for a conversation or collaboration!







By PhD student Anne Laustsen: Furry mask Molecular dynamics (MD) simulation of 200 sodium dodecyl sulphate (SDS) molecules each in different colours. Only the twelve carbon-tail is included for SDS. Water is not shown.

# HIGHLIGHTS 2013 & 2014



#### TWO INANO SCIENTISTS HANDED THEIR AWARDS AT ELITE RESEARCHER CEREMONY 2014

At a ceremony that took place in the beautiful Ny Carlsberg Glyptotek, Prof. Daniel Otzen received the EliteForsk (Elite researcher) award from the Danish Agency for Science, Technology and Innovation. The award is a grant of DKK 1.2 million. Prof. Otzen received his award for his major contributions to the understanding of proteins and in particular protein folding. He was one out of five researchers to receive the award.

In addition PhD student Signe Korsager was one out of twenty PhD students to receive the Eliteforsk travel scholarship.



#### INANO RESEARCHERS REVEAL A NEW METHOD TO MAKE HYDROGEN FROM WATER

Catalysts made of molybdenum sulfides have been used for the desulphurisation of oil since World War II. Dr. Jakob Kibsgaard has now revealed promising results to produce hydrogen from water by means of nanoparticles of Mo3S13 in a collaboration between the universities in Aarhus and Stanford. The Mo3S13 nanocluster can be produced cheaper and easier than conventional alternatives.

#### CDNA PhD STUDENT PUBLISHES IN NATURE BIOTECHNOLOGY

PhD student Christian Bech Rosen shows how a protein nanopore can be used to discriminate between different phosphorylation states of a protein at the single-molecule level. The results provide a step toward nanopore proteomics.



#### INANO RECEIVES TWO VILLUM FOUNDATION YOUNG INVESTIGATOR GRANTS

Dr. Nina Lock received DKK 3.9 million for her project on functional hybrid materials. These materials can use sunlight to drive chemical reactions such as the electrolysis of water into hydrogen and oxygen. Dr. Dorthe Ravnsbæk received DKK 3.8 million to her project on the development of batteries. The overall goal will be to develop rechargeable batteries that are cheaper and more efficient than the current Li-ion technology. These batteries will be based on cheap materials such as Mg and Al.



#### FLEMMING BESENBACHER RECEIVES NEW RECOGNITION FROM CHINA

Professor Flemming Besenbacher was appointed foreign member of the Chinese Academy of Sciences (CAS), which provides consultancy services for the Chinese government.

Flemming Besenbacher has joined China's most exclusive scientific league, consisting of 750 Chinese and 72 foreign scientists, including several Nobel Laureates. It is considered the highest scientific position a foreigner can achieve in China.



### STUDENTS WIN THE HEARTS OF THE AUDIENCE WITH NANOMEDICINE

A team of Aarhus students - Nano Creators - won the Audience Choice Award for their Bachelor's project at Harvard University's bio-molecular design competition. The Nano Creators combined good research with creative communication.



### CRUCIAL NEW INSIGHT INTO THE SECRETS OF NOBEL PRIZE-WINNING PUMP

Jens Chr. Skou was awarded the Nobel Prize for his discovery of the sodium-potassium pump. Now, a team of researchers from iNANO has completed the description of its structure and publised it in Nature. A result which is of vital importance for our understanding of the body's functions and essential for our understanding of illness and for the development of new medicines.



#### PROFESSOR KIM DAASBJERG AWARDED THE ELASTYREN PRIZE 2013

Professor Kim Daasbjerg, iNANO and Department of Chemistry, was awarded the Elastyren Prize 2013 by the Danish Academy of Technical Sciences (ATV).

Professor Kim Daasbjerg received this prestigious award in recognition of his groundbreaking research on surface-bound polymers. The award was presented at the Annual Meeting of the Danish Academy of Technical Sciences on 18 April 2013. With the award follows a prize of DKK 100,000.



#### NANO STUDENTS TAKE HOME THE GLOBAL GRUNDFOS CHALLENGE 2013

Three iNANO students, Signe Grønborg, Irene Hansen, and Simon Frølich, won the Global Grundfos Challenge in Engineering – an award worth DKK 75.000. The students received the award for their water network solution. The solution deals with the implementation of various sensors, including a novel sensor for detecting bacteria.



#### NEW KNOWLEDGE ABOUT THE HUMAN GENOME

iNANO researchers have discovered a completely new function in human cells. In the long term, this could be very significant for understanding and treating a considerable number of human diseases. The results, which were published in Nature, describe the function of a circular RNA molecule, cirRS-7 (circular RNA sponge for miR-7), which is capable of blocking the function of other RNAs.



### THREE INANO SCIENTISTS WIN THE VENTURE CUP IDEA COMPETITION

Dr. Ryosuke Ogaki, PhD student Kristian Kolind and Senior Scientist Morten Foss from the Biomedical Surface Group won this year's Venture Cup Idea competition in the Life Science & MedTech category. Venture Cup is an entrepreneurship competition aiming to identify the most promising ideas and research results with a strong business potential.



#### PROFESSOR BO BRUMMERSTEDT IVERSEN AWARDED THE GRUNDFOS PRIZE 2014

The prize was awarded to Prof. Iversen for his work on thermoelectric materials, which offer the possibility of a more efficient use of waste heat.



#### PROFESSOR TROELS SKRYDSTRUP SECURES A NEW CENTER OF EXCELLENCE

As the only unit of Science and Technology, iNANO won a new Center of Excellence from the Danish National Research Foundation. Headed by organic chemist, Professor Troels Skrydstrup, the "Carbon Dioxide Activation Center" (CADIAC) aims at developing new and efficient catalytic systems for converting  $CO_2$  into high-value compounds.



#### INANO RECEIVES FOUR GRANTS FROM THE DANISH INNOVATION FUND

During the first granting round of the new Danish Innovation Fund, iNANO secured as much as four new grants. Associate Professor Rikke Louise Meyer, Professor Kurt Vestrager Gothelf, Associate Professor Kenneth Alan Howard, and Senior Researcher Morten Foss all joined with industry to carry out research aimed at solving concrete problems in the partner companies.



#### COMMISSIONING OF NEW STATE-OF-THE-ART ELECTRON MICROSCOPES

Towards the end of 2014, iNANO commissioned additional three new electron microscopes. In particular, the FEI Talos with Electron Energy Loss Spectroscopy capabilities represents a large step up in our capabilities to atomically resolve and chemically identify hard and soft materials.



#### PROFESSOR JØRGEN KJEMS APPOINTED DIRECTOR FOR THREE YEARS

As of 1 January 2015, Professor Jørgen Kjems was appointed director of iNANO. Prof. Kjems has been involved in iNANO since the very beginning in 2002, and he already served as interim director in 2014, so his appointment ensures continuity and a world-class researcher at the helm of iNANO.

# INANO INFRASTRUCTURE PLATFORMS

To support research within our three strategic research areas, iNANO has established three infrastructure platforms with focus on synthesis, characterization, and modelling. These platforms have been established as universal infrastructure supporting research within prioritized areas, but the uniqueness of several instruments forms an extremely powerful platform for international collaborations and recruitment.  iNANO welcomes external users, existing project partners, or prospective new partners from academia and industry.

# THE DANISH CENTER FOR **ULTRAHIGH-FIELD NMR SPECTROSCOPY**

# **ELECTRON** MICROSCOPY



The Danish Center for Ultrahigh-Field NMR Spectroscopy was established in the beginning of 2015 as a national/Scandinavian center with state-of-the-art NMR equipment for solid- and liquid-state NMR and micro-MRI, including Northern Europe's largest (950 MHz/22.3 Tesla) NMR magnet. The center hosts the internal research groups headed by Jørgen Skibsted, Niels Christian Nielsen, Frans Mulder, Umit Akbey, Anders Bodholt Nielsen, Michael Ryan Hansen, and Thomas Vosegaard. These research groups are internationally established within the structure and dynamics of insoluble proteins (N. C. Nielsen, T. Vosegaard, U. Akbey), intrinsically disordered proteins (F. Mulder), low-temperature hyperpolarization (A. B. Nielsen), concrete/ materials (J. Skibsted), and polymers (M. R. Hansen). In addition to the internal activities, the center invites academic and industrial collaborators from Denmark and the rest of Scandinavia to carry out experiments on its instrumentation at iNANO.

For further information, please contact **Thomas Vosegaard** tv@chem.au.dk



iNANO also commands an advanced array of electron microscopes. For biological studies, we have set up an imaging pipeline involving a Tecnai Spirit TEM and a Titan Krios TEM with automated image acquisition. The Titan Krios is equipped with an image Cs corrector and is hence also suitable for imaging of hard materials at atomic resolution. Most recently, a Talos TEM was added to the suite. The Talos has a unique configuration, which includes a very powerful Bruker X-ray analysis system and a Gatan EELS analyzer for qualitative and quantitative chemical characterization. In addition, we host a number of more conventional instruments, such as a dual-beam SEM with Focused Ion Beam capabilities for TEM sample preparation, a Magellan SEM with e-beam lithography and a NOVA SEM with Energy Dispersive System.

Our electron microscopes are open to all users, including external academic and industrial users.

For more information, please contact **Jacques Chevallier**, jach@phys.au.dk

# **CHARACTERIZATION**







Nanoindentation and Ion Scattering.

#### NANOANALYSIS

iNANO commands a wide variety of analytical instruments for the elucidation of nanostructures and functions at high resolution. These include: (STM) Scanning Tunneling Microscopy Atomic Force Microscopy (AFM) (SAXS) Small Angle X-ray Scattering Spectroscopy X-ray Photoelectron Spectroscopy (XPS) (XAS) X-ray Absorption Spectroscopy High-Field Liquid- and Solid-State Nuclear Magnetic Resonance (NMR) High-Field Magnetic Resonance Imaging (MRI) (TEM/SEM) Transmission and Secondary Electron Microscopy (XRD) Cryo-TEM, X-ray Crystallography (MS) Mass Spectrometry IVIS in vivo imaging (Optical imaging) Time-of-Flight Secondary Ion Mass Spectrometry (ToF-SIMS) Thermal Analysis, Quartz Crystal Microbalance (QCM) Surface Plasmon Resonance (SPR) Physical Property Measurements (PPMS)

For detailed descriptions of these instruments and their capabilities, please refer to www.inano.au.dk

A number of these instruments are unique in a Danish and Nordic context; for instance, the world-famous "Aarhus STM" was developed at iNANO, and the recently purchased Cryo-TEM is the highest resolution instrument of its kind in Scandinavia.

In 2011, the Danish Roadmap for Research Infrastructure promoted the establishment of a Danish-Scandinavian ultra-high field NMR instrumentation center at iNANO. This involves the installation of one of the most powerful NMR instruments in the world, a 950 MHz NMR machine.





STM



ToF-SIMS



Cryo-EM





**ACCESS FOR EXTERNAL** INDUSTRIAL AND ACADEMIC USERS

iNANO welcomes external users. Many of our analyses are carried out in collaborative projects, but we also offer analyses for paying users.

For contact information, please refer to our homepage www.inano.au.dk



 $\diamond$ 

# **SYNTHESIS**

iNANO has invested and continues to invest large resources in the establishment of a platform for nanoscale synthesis with relevance for materials science, medicine, and food-related interdisciplinary projects. This involves areas of organic chemistry, protein chemistry, and nucleic acid chemistry, self-assembly of nanostructures, nanoparticle formulations, etc., in addition to cultivation and analysis of cells and bacteria. The 120 m<sup>2</sup> class-100 cleanroom research facility enables the fabrication of nanostructured materials and devices with state-of-the-art lithography resolution. It houses all the necessary equipment for silicon processing, including wet benches, mask aligner, furnace, sputter deposition, scanning electron microscopy, and plasma-enhanced physical vapor deposition.



Fibril The image depicts the atomic structure of an amyloid fibril composed of NFGAILS peptides. (PDB-ID: 24XIB) The image has been rendered with VMD.

# NANOMODELLING

To complement analysis and form models for phenomena at the nanoscale, iNANO is currently working with modelling activities spanning from materials to biological macromolecules and from high-resolution structural models to 3D video animations. Such methods are highly valuable to obtain detailed insight into complex multicomponent systems for research as well as for education and outreach activities which rely heavily on visualization.

#### INANO VISUALIZATION LAB

The Visualization Lab offers a research programme for optimizing scientific data design and scientific imagery in contemporary bio- and nanoscience. The rapid increase of molecular and nanoscale data in contemporary science has produced an urgent need for the development of new visual frameworks and tools to explore, analyze and communicate data. The Visualization Lab makes scientific imagery a concerted interdisciplinary effort at Aarhus University. Through critical assessment of tools and methods, and the investigation of the dissemination, semiotics, and reception of scientific visual representations, the Visualization Lab produces workable graphic solutions for bio-nanoscience data.

The Visualization Lab develops innovative visual solutions for contemporary scientific imagery, creates integrated visual systems based on graphic design and animation, and develops educational strategies in science visualization for scientists.

The main objects of the Visualization Lab is to produce a new graphic standard framework for molecular and nanoscale science; and to develop exploratory 3D animations specific for bio-nanoscience data analysis using high-end 3D software initially developed for the art and entertainment industry.

# **OVERVIEW** OF INANO SENIOR RESEARCHERS

Umit Akbey	Structural Biology, Solid-State Nuclear Magnetic Resonance (NMR) Spectroscopy, Dynamic Nuclear Polarisation (DNP), Functional Amyloids, Bacterial Biofilms and Infections
Ebbe Sloth Andersen	DNA Nanotechnology, Molecular Self-Assembly, Molecular Biology, Biophysics, Synthetic Biology
Peter Andreasen	Serine Proteases, Serpins, Protein Structure-Function Relationships, Regulatory Agents, Cancer
Peter Balling	Ultrashort-Pulse Lasers, Ultrafast Material Excitation, Solar Cells, Upconversion, Semiconductors
Emøke Bendixen	Metagenomics, Pig Models, Gut Bacteria, Proteomics, Immunology
Henrik Birkedal	Biological Materials, Bioinspired Materials, Nanocrystals, X-Ray Scattering and Imaging, Synchrotron
Victoria Birkedal	Nanoscale Biophysics, Nucleic Acids, Structural Dynamics, Fluorescence Spectroscopy and Microscopy, Single Molecule Microscopy
Martin Bremholm	Crystallography, Solid State Chemistry, High Pressure, Crystal Growth, Functional Materials
Menglin Chen	Electrospinning, Nanofibers, Extracellular Matrix, Tissue Regeneration, Drug Delivery
Mogens Christensen	Neutron Scattering, X-Ray Diffraction, Magnetism, Energy Materials, Crystallography
Mingdong Dong	Atomic Force Microscopy, Nanomechanics, Nanomaterials, Bioimaging, Surface Science
Kim Daasbjerg	Carbon Dioxide, Graphene, Polymer Brushes, Materials Science, Electrochemistry
Jan Enghild	Protein Chemistry, Proteomics, Extracellular Matrix Homeostasis, Coagulation and Fibrinolysis, Corneal Diseases
Elena Ferapontova	DNA Electronics, (Photo)Electrocatalysis, Electron Transfer in Proteins, Medical and Environmental Biosensors, Biofuel Cells (Energy Research)
Morten Foss	Biomedical Surfaces, Implants, Non-Fouling Coatings, Large-Scale Screening, Micro- and Nanofabrication
Marianne Glasius	Chemical Analysis, Atmospheric Chemistry, Mass Spectrometry, Biofuels, Aerosols
Kurt Gothelf	DNA, Organic Synthesis, Self-Assembly, Bioconjugation, Biosensors
Bjørk Hammer	Theory of Chemical Bonds, Surface Science, Asymmetric Catalysis, Heterogeneous Catalysis, Density Functional Theory (DFT)
Michael Ryan Hansen	Solid-State NMR, Conjugated Polymers, Co-Polymers, Organic Solar Cells, Graphene-Based Nano-Composites
Megan Ho	DNA Nanosensors, Microfluidics, Fluorescence Spectroscopy, Enzymatic Activities, Single Cell Dynamics
Liv Hornekær	Scanning Tunneling Microscopy, Graphene, Functionalized Surfaces, Graphene Coatings, Band Gap Engineering
Ken Howard	Nanomedicine, Surface Engineering, Polymers, RNA Interference, Inflammatory Diseases
Bo Brummerstedt	Materials Crystallography, Energy Materials, Synchrotron Radiation, Neutron Scattering, Supercritical Fluids
Torben Jensen	Inorganic Nanomaterials, Hydrogen Storage, Nanoconfinement, Nanoporous Materials, Gas Adsorption,
Jan Kristian Jensen	Serine Proteases and Inhibitors, Multidomain-Functionality, Protein-Modulators, Tertiary Structure, Biochemistry
Brian Julsgaard	Light Emission, Silicon, Group-IV Photonics, Nanostructures, Time-Resolved Spectroscopy
Søren Keiding	Femtoseconds, Optical Tweezers, Supercontinuum, Spectroscopy, Water
Jørgen Kjems	Non-Coding RNA, RNA Interference, Tissue Engineering, Drug Delivery, Bioimaging

Rikke Schmidt Kjærgaard	Data Visualization, Molecular Animation, Visual Communication, Information Design, Visual Analysis
Magnus Kjærgaard	Single Molecule FRET, Protein Dynamics, Membrane Proteins, Intrinsic Disorder, Neuroscience
Birgitta Knudsen	Biosensors, Enzymes, Diagnosis, Single-Molecule Detection, Disease
Arne Nylandsted Larsen	Semiconductors, Solar Cells, Epitaxy, Defects, Plasmonics
Jeppe Vang Lauritsen	Catalysis, Surfaces, Scanning Probe Microscopy, Surface Science, Energy Materials
Trolle Linderoth	Surface Science, Scanning Tunneling Microscopy, Molecular Self-Assembly, Dynamic Surface Processes, Surface Chirality
Nina Lock	Hybrid Materials, Porous Materials, Structure-Property Relationship, Catalysis, Optical Properties
Rikke Meyer	Biofilms, Bacterial Adhesion, Single-Cell Interactions, Antimicrobial Compounds, Antifouling Surfaces
Frans Mulder	NMR Spectroscopy, Biophysics, Protein Dynamics, Protein Electrostatics, Structural Biology
Arne Möller	Electron Microscopy, Cryo-EM, Single Particle Analysis, Membrane Proteins, Structural Biology
Lene Nejsum	Water Balance, Kidney, Aquaporins, Urine Concentration, Imaging
Poul Nissen	Membrane Proteins, Transporters, Crystallography, Structural Biology, Drug Discovery
Jens Vinge Nygaard	Biomechanics, Biomaterials, Materials and Tissue Engineering
Daniel Otzen	Protein Aggregation, Functional and Pathological Amyloid, Protein-Fatty Acid Complexes, Membrane Protein Folding, Protein-Biosurfactant Interactions
Jan Skov Pedersen	Molecular Self-Assembly, Responsive Systems, Drug Delivery, Structure, Small-Angle X-Ray Scattering
Birgit Schiøtt	MD Simulation, Protein Modelling, Protein-Lipid Interactions, Amyloid Diseases, Lipid Membranes
Jørgen Skibsted	Solid-State NMR, Portland Cement, CO, Emission, Heterogeneous Catalysis, Materials Research
Troels Skrydstrup	Catalysis, Organic Synthesis, Carbon Dioxide, Pharmaceuticals, Isotope Labeling
Brigitte Städler	Artificial Cells/Organelles, Droplet Microfluidics, Liposomes, Poly(Dopamine), Self-Propelled Swimmers
Duncan Sutherland	Nanofabrication, Functional Materials, Biosensors, Plasmonics, Nanotoxicology
Thomas Vorup-Jensen	Immunology, Autoimmune Diseases, Biophysics, Structural Biology, Nanoscience.
Thomas Vosegaard	Nuclear Magnetic Resonance (NMR) Spectroscopy, Danish Center for Ultrahigh-Field NMR Spectroscopy, Structure and Dynamics of Insoluble Proteins, Protein-Lipid Interactions, NMR Method Development
Stefan Wendt	Model Catalysis, Oxide Surfaces, Titanium Dioxide (TiO <sub>2</sub> ), Scanning Tunneling Microscopy (STM), Temperature-Programmed Desorption (TPD)
Alexander Zelikin	Polymers, Hydrogels, Prodrugs, Antiviral Therapy, Enzyme Prodrug Therapy

# MESSAGE FROM THE CHAIRMAN

I take great pleasure and pride in writing this message in support of the excellent work done at the Interdisciplinary Nanoscience Center, iNANO. It is an organization whose merits and aspirations are wellknown all over the world and iNANO is such a strong brand that it should, and indeed is, used to draw attention to Aarhus University. The iNANO board consists mainly of industrial representatives from major Danish companies, who have all taken part in collaborative projects with iNANO researchers. We lend strategic advice to the iNANO management on both educational, scientific, and innovation activities and miss no opportunity to promote iNANO in our daily work. We do so because we feel that iNANO has found a concept which facilitates the sort of close interaction with industry that is highly desirable not only to strengthen industrial competitiveness but also to help meet some of the daunting Grand Challenges faced by the world today. History shows that iNANO often serves as a portal to finding the right academic partners in such ventures, especially when an interdisciplinary team is needed.

iNANO is such an attractive partner because of its strong foundation in basic research. In fact, I feel that it is important that academic researchers spend just as much time on fundamental research as on strategic/applied research as the methodology and level of abstraction necessary to do frontier basic research carries over extremely well to more applied projects.

Finally, let me express my full support to the new concept of a biannual iNANO profile. The board feels that it will serve the honorable purpose of promoting iNANO and its excellent activities to existing and new academic and industrial alike.

### The iNANO board consists mainly of industrial representatives from major Danish companies



#### **Board Members**

**Bjerne Clausen,** CEO, Haldor Topsøe A/S (Chairman of the board)

Hans Jørgen Pedersen, CEO, Flowsion ApS

Charlotte Poulsen, Enzyme Development Director, DuPont

Lars Enevoldsen, Group Vice President, Global Research & Technology, Grundfos A/S

Henrik Jørgen Andersen, Senior R&D Manager, Arla Foods Ingredients Group P/S

> Jan Egebjerg Jensen, Divisional Director, Lundbeck A/S

Niels Chr. Nielsen, Dean, Faculty of Science and Technology, Aarhus University

> Allan Flyvbjerg, Dean, Faculty of Health Sciences, Aarhus University

**Eskild Holm Nielsen,** Dean, Faculty of Engineering and Science, Aalborg University

# **SPIN**OUT



NAME SyTracks A/S

#### FOUNDERS

Prof. Dr. Troels Skrydstrup, Dr. Rolf H. Taaning and Dr. Anders T. Lindhardt.

#### **BUSINESS AREA**

SyTracks specializes in the simple and safe handling of gaseous reagents in organic synthesis. Their technology and reactor hardware covers synthesis in research and development, early stages of scale-up and isotope labeling. Besides know-how based services, SyTracks also holds a well-established catalogue of technologyderived chemicals and provides special chemical building blocks on request to both industry and university research. Key collaborators: Sigma-Aldrich and Manchester Organics.

Website: www.SyTracks.com

**NAME** LevOss Aps

#### FOUNDERS

Lea Bjerre, Cody Bünger, Flemming Besenbacher and Jens Vinge Nygaard

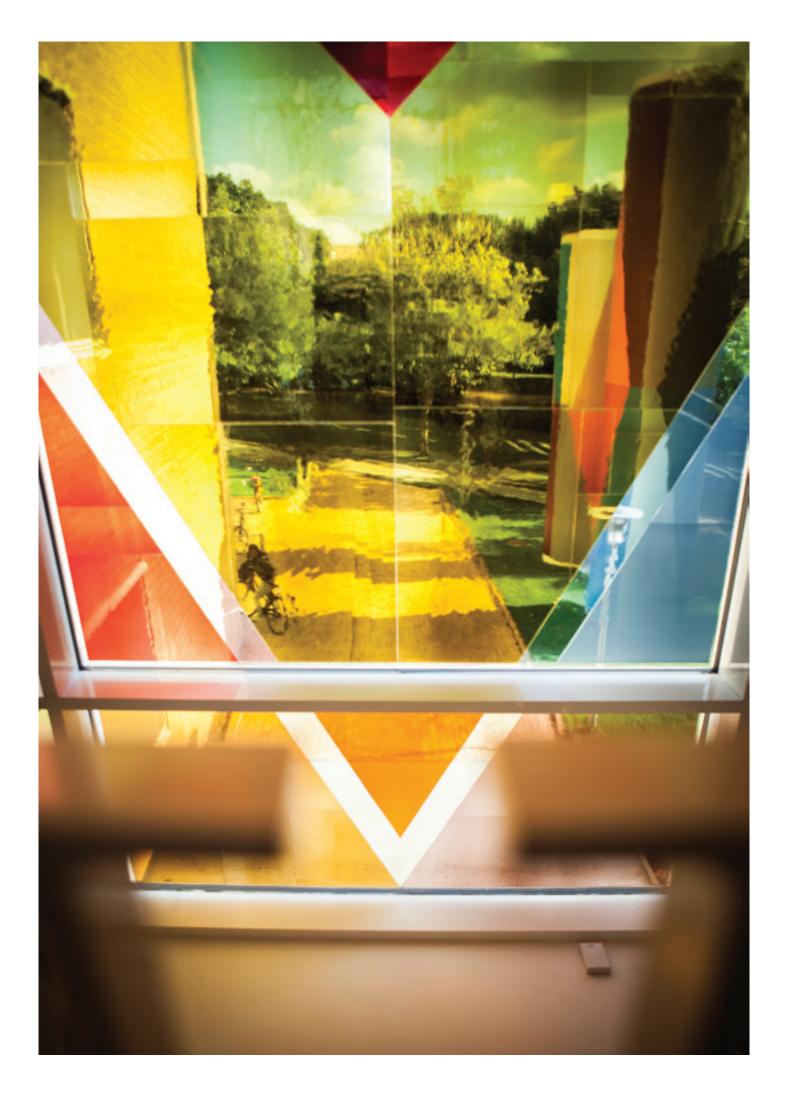
#### **BUSINESS AREA**

Biotechnology - technologies for mechano transduction

LevOss has developed an implant device, a scaffold, that supports the regeneration of lost tissue - with current primary focus on cartilage and bone regeneration.



Website: www.levoss.com



# **INANO** MANAGEMENT AND ADMINISTRATION



#### Jørgen Kjems Peter Thostrup Yvonne Eskildsen-Helmond - Scientific coordinator Annette Wandahl Trine Møller Hansen Rebeca Thostrup Maria Kragelund

- Director
- Vice director
- Head of secretariat
- Administrative officer
- Administrative officer
- PhD administrator

Starting from the top left: Annette Wandahl, Trine Møller Hansen, Peter Thostrup, Yvonne Eskildsen-Helmond, Maria Kragelund and Rebeca Thostrup



CONTACT PERSON Maria Kragelund Phone: +45 2118 4164

Aarhus University Science and Technoloc

iNANO – Interdisciplinary Nanoscience Center Gustav Wieds Vej 14 8000 Aarhus C

