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Nano-Science Center

The Nano-Science Center with the University of Copenhagen is one the world’s leading research environments for nanoscience. More than 200 researchers from classical research areas like physics, chemistry, biology and medical sciences are members of the center linking the Faculty of Science and the Faculty of Health and Medical Sciences. The broad range of research groups in the Nano-Science Center each bring in high-level expertise in various areas of theory, experimental methods and instrumentation into joint research projects and into the nanoscience degree programme. In September 2001, the center was inaugurated as a joint venture between the Niels Bohr Institute and the Department of Chemistry at the University of Copenhagen. The center was the first in Denmark to introduce a full bachelor and master’s programme in nanoscience. Today, the center has approx. 250 students. Many of our candidates choose to do a PhD; others make careers in industry. It has been 15 years since the first nanoscience students in Denmark started their studies at the Nano-Science Center. According to Ministry of Higher Education and Science, holders of an MSc in nanoscience have one of the highest employment rates in Denmark, corresponding to 2% of the candidates from 2010 being unemployed in the first two years after their graduation, www.ufm.dk.

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In the Nano-Science Center, we have over the years developed our unique approach to research and education in nanoscience. This ‘Copenhagen nanoscience’ has become an inspiring platform that attracts creative researchers and students. I am proud to see the many new research projects and collaborations established by our researchers and the skilled MSc and PhD graduates trained in the Nano-Science Center.

Bo Wegge Laursen
Professor
Director of the Nano-Science Center
2017 in short

Highlights of the Nano-Science Center activities include:

- The nanoscience undergraduate and master’s programme both enrolled 49 students in September.

- A total of 7 companies participated in our annual Science Dating in November, an event where we invite businesses to spot nanoscientific talent among our undergraduate and graduate students. In the name of networking, our students met the companies to talk about career and how to use nanoscience in industry.

- In August, the Nano-Science Center co-hosted the 8th international symposium on carbon nano materials and 2D materials: Carbonhagen together with DTU Nanotech and reached a total of 160 participants in 2017. Read more at http://www.carbonhagen.com

- New tenure-track Assistant Professor Maria Escudero Escribano was recruited from Stanford University, California, USA to form the new group Nano Electro catalysis. Her group investigates electrochemical interfaces for energy conversion reactions and electrocatalytic synthesis of fuels and chemicals.

Happy reading
Bo Wegge Laursen, Director, and Tine Buskjaer Nielsen, Center Coordinator
Nano-Science Center has since 2013 offered a two-year master’s programme in nanoscience and technology at the Sino-Danish Center for Education and Research (SDC) in Beijing.

SDC is a partnership between all eight Danish universities, the Chinese Academy of Sciences (CAS) and the University of Chinese Academy of Sciences (UCAS).

The overall objective is to promote and strengthen collaboration between Danish and Chinese learning environments and increase mobility of students and researchers between Denmark and China.

SDCs activities include Danish-Chinese research collaboration in five selected focus areas, seven affiliated master’s programmes with an annual intake of approximately 150 master’s students and training of a large number of PhD students. All graduates will obtain a double degree from both the University of Chinese Academy of Sciences and one of the Danish partner universities.

Sino-Danish Center is located at UCAS' Yanqihu Campus north of Beijing at the “The House of the Danish Industry Foundation” designed by Danish Lundgaard & Tranberg Architects.

Academic staff and researchers at the Nano-Science Center, UCPH, iNano, Aarhus University and National Center for Nanoscience and Technology (NCNST), UCAS, are responsible for the majority of the teaching of the courses. This includes an overlap with researchers who have collaborated for more than ten years.

The first year consists of class teaching and exercises in the laboratory at the NCNST while the second year will focus on the thesis. Besides the nanoscience classes, students will also be introduced to Chinese language.

In the class of 2017, 9 Danish/International and 13 Chinese students were enrolled, of which three were semester students.

Questions? Contact programme cooordinator Vibe Thybo Drostgaard v.drostgaard@nano.ku.dk
New marking technique could halt counterfeit goods

Researchers at the University of Copenhagen have developed the world’s most secure marking system for combating pirated goods including pirated pharmaceuticals, foodstuffs, designer merchandise and artwork. The system could be on the market in a year and because the markings are random, it cannot be hacked. The results have just been published in Science Advances, a scientific journal.

Companies around the world consistently suffer significant economic losses due to counterfeited goods made by pirate manufacturers for whom international patents are of no concern. Nor do these pirates lose sleep over placing people’s lives at risk when they sell dangerous and counterfeit medications online. However, tough times are on the horizon for pirates according to four researchers from the Nano-Science Center. They have developed a system that head of research and Associate Professor Thomas Just Sørensen calls “the safest in the world” when it comes to clamping down on all types of pirate manufacturing:

“The system, which deploys three rare earths among other things, is based on randomness, which makes it unable to be hacked or tampered with”, says Thomas Just Sørensen:

“As soon as a customer asks that an authorized dealer checks up on a piece of merchandise that was meant to be marked using the system, an expensive wrist watch for example, the dealer can access a manufacturer database to check its authenticity.”

Can be on the market in a year

The University of Copenhagen has taken out a patent on the marking system and it is expected to be on the market in roughly a year. Researchers are currently fine-tuning scanning solutions to ready the system for manufacturers. According to Thomas Just Sørensen:

“We estimate that it will take approximately one year, at which point we will be very close to being able to put a commercial version on the market.”

Researchers estimate that the cost of marking products will be modest, probably not much more than one Danish krone. Additional expenses from the data systems have yet to be fully estimated.

The probability of two products having the same ‘fingerprints’ – the same digital key – is so minuscule, that in practice, it can only be described as non-existent, It corresponds to a one out of an enormous number composed of a 6 followed by 104 zeros.”

Thomas Just Sørensen
Associate Professor and member of Nano-Science Center

The article in Science Advances can be accessed here:
http://advances.sciencemag.org/content/4/1/e1701384/tab-e-letters
DKK 60 million for developing super-cells

Researchers at University of Copenhagen will use light to develop super-cells that are more effective at fighting cancer and a wide range of other serious diseases. This has been made possible with a new six-year research grant from the Novo Nordisk Foundation.

The human body is made up of billions of cells that may potentially develop into severe diseases such as cancer. In order to adapt, grow and reproduce, the cells consist of innumerable molecules that are organized in very precise patterns. These patterns not only determine the function and survival of the cell, they are also the focus of a six-year research project that has just been granted DKK 60 million from the Novo Nordisk Foundation Challenge Programme.

“We are embarking on a new direction that will expand our understanding of cells and our ability to control their behavior. It has the potential to become a breakthrough but at such an early stage uncertainty is high. The actual potential and added value will become more concrete over the next six years through our intense research efforts.,” says the professor heading the research project, Dimitrios Stamou from the Nano-Science Center.

Super immune cells

The results of Dimitrios Stamou’s research are potentially far-reaching as regards the way the health sector will be able to treat severe diseases such as diabetes, Alzheimer’s, cardiovascular diseases, fertility diseases and cancer.

”By redesigning the molecular patterns in the cell, we can make the cell behave the way we want. One possibility may for instance be to develop super immune cells that will kill cancer cells more effectively before they become a tumor”, says Professor Dimitrios Stamou, who collaborates with researchers from University of California, Berkeley, and School of Medicine, University of California, USA.

Light beams may control the cell

To redesign the patterns of molecules in a cell, researchers will apply different methods, including what is called ‘optogenetics’ whereby special light beams can be used to make the molecules place themselves in new patterns, thus allowing the researchers to control the behavior and function of the cell. A method that is not yet widespread but is very promising.

According to Dimitrios Stamou, the development of super immune cells has a time horizon of more than ten years before the method can be tested on humans.
Origin of life

Researchers at the University of Copenhagen have found the earliest traces of life encapsulated in 3.7 billion-year-old gems found in Greenland.

The discovery was made using a novel method allowing the research team to examine and prove the minute quantities of carbon was the ancient material originating from the earliest life forms. The results have been published in Nature and yields exciting possibilities for the future investigation of the origin of life, e.g. on Mars or other places which may have supported life in the past.

Behind the study we see Associate Professor Tue Hassenkam from the Nano-Science Center and Professor Minik Rosing from Natural History Museum of Denmark at University of Copenhagen.

Read the article in Nature:
https://www.nature.com/articles/nature23261
ARTiS - Art in Science

The ARTiS: Art in Science is the outreach programme of University of Copenhagen meant to use art to communicate science to a broad audience. This includes an original approach to educate and engage children in scientific disciplines. It is furthermore a unique opportunity for scientists to talk about their work in an original context.

ARTiS 2017 was composed of the yearly picture contest, children boot camps and the yearly picture exhibition. About 100 pictures were part of the picture contest 2017 attracting 3,500 people to the ARTiS 2017 exhibition in the ceremonial hall of University of Copenhagen during Culture Night. This programme is headed by Karen L. Martinez, associate professor and head of the BioMeP group. It has been sponsored by Lundbeckfonden and University of Copenhagen.

ARTiS Prizes 2017

1st prize 2017
“Beauty in seawater” by Jannicke Wiik-Nielsen, Norwegian Veterinary Institute.

Young Art-scientist Prize 2017
“Flower” by Andrii Lapytskyi

Children boot camp 2017
Illustration of the Agar Art activity – painting with bacteria.

Karen L. Martinez
Head of ARTiS
A year full of prices!

Three young researchers at the Nano-Science Center, have received grants from the Villum Foundation. The projects point towards a greener and environment friendly world.

Jiwoong Lee: Water: Divide and Conquer (Split and Purify)
Water is the most important molecule on Earth. All forms of life consist of water, which also provides the essential environment for proliferation of life. However, recent global climate change is seemingly accelerating the unpredictability of secure water supply sources. This project will provide a new Catalytic Desalination Process by Diamine and Carbon Dioxide. The grant will fund two PhD students and one postdoc.

Maria Escudero Escribano: Atomic ensembles for clean energy and synthesis
Electro catalysis is essential for the development of a green economy based on clean energy and sustainable chemical synthesis. The main purpose of Atom-Syn is to understand and tune the selectivity of new “dream” electrochemical reactions by atomic-scale control of the geometric structure of the catalyst surface. This approach will allow us to convert greenhouse gases into fuels as well as synthesise high-value chemicals. The grant will fund three PhD students, two postdocs and equipment.

Vito Foderà: Protein Superstructures as Smart Biomaterials (ProSmart)
Protein superstructures hold a great potential as new biomaterials in areas such as tissue engineering and drug delivery. This project aims at unravelling the role of intermolecular interactions in controlling the growth, structure and properties of protein superstructures. The project will provide a novel platform for the design and realisation of tailored protein-based materials. The grant will fund two postdocs, one PhD student and equipment.
Microsoft and researchers cooperate to develop and build the first general-purpose quantum computer

We live in a world full of computers, where everything is done on computers, even research is rarely done without. Today, programming can solve various problems as simple molecule structures and properties, but often the research is limited by computer power. In this perspective quantum computers would push the boundaries and open the possibilities for more advanced systems to explore in modern research.

In modern computers, the bit system is used where the state can only be 0 or 1. This is optimized in quantum computers, where qubits are used. In the quantum world, the spin state of an electron can have the state 0 and 1 simultaneously, which means that the state can be a linear combination of these two. By taking advantage of this technique, the quantum computer would have plentiful states increasing the computer power significantly.

For several years, Microsoft has been collaborating with world-leading scientists in the field of quantum computing from the research group Qdev. The vice-director of the Nano-Science Center, Jesper Nygård, is in charge of the material synthesis in Qdev. In the mandatory course, Quantum Phenomena in Nano Systems, he gives the students an introduction to experimental nano electronics. Therefore, both students and researchers from Nano-Science Center will benefit from the cooperation.

In 2017, the partnership was expanded making Copenhagen one of the world-leading capitals of quantum mechanics. With this expansion, Microsoft is establishing state-of-the-art laboratories and several employees will be based in Universitetsparken 5. Hopefully the new phase of the collaboration will create a foundation for a paradigm shift in the computer technology.
Publications & Citations

In 2017, researchers from the Nano-Science Center successfully published more than 145 peer-reviewed papers. Their works were cited more than 11,500 times.

*Publications from Nano-Science Center researchers during the last 20 years.*

*Citations of Nano-Science Center researchers during the last 20 years.*
Outreach

Outreach is key to the Nano-Science Center in relation to recruiting new students and communicating with external stakeholders such as businesses.

NanoKits
At several occasions, for instance conferences for school teachers, our NanoKits have been demonstrated by Nano-Science Center facilitators. NanoKits are experiment kits targeted pupils in lower secondary school, 8th and 9th grade, showing nanoscience in practice.

Recruiting events
Open House for potential nanoscience students.

Presentations for high school students visiting the Nano-Science Center with their physics or chemistry classes.

Field-of-study projects
Total of 12 students from high schools visited the Nano-Science Center for three days to make experiments for their field-of-study project.

Student trainees
A high-school promotion event where 20 high-school students visit Nano-Science Center for three days doing experiments, attending lectures and socializing with nanoscience students.

Science Dating
Where students meet representatives from industry. Seven Danish companies participated in our annual Science Dating in November, an event where we invite businesses to spot nanoscientific talent among our undergraduate and graduate students. In the name of networking, our students met the companies to talk about career and how to use nanoscience in industry.
External Funding

During 2017, the research groups in the Nano-Science Center received funding from national and international funding agencies and private foundations.

![Graph showing funding from different sources over the years.]

External Relations

Collaboration with the private sector comes in different shapes and sizes: consulting, commissioned research, shared student projects on BSc, MSc and PhD level or research projects that are fully or partly funded by a business. Selected partners in 2017:

- DONG Energy
- Reykjavik Energy
- Rockwool
- Haldor Topsøe
- NIL Technology
- Niras
- COWI
- GEO
- Applied Biomimetic
- BMW
- Novo Nordisk
- Microsoft
- Gubra aps
- Novartis
- Quantumwise
- Hempel
- Medtronic
- Novozymes
- DFM A/S
## Graduated PhDs in 2017

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<td><strong>Sofie Cecilie Fogh Hedegaard</strong></td>
<td>Hydrophobic tailoring of peptide and proteins in drug delivery - Membrane interactions and adsorption behavior</td>
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Research groups
The BioMEP group, headed by Karen L. Martinez focuses on the investigation of G Protein Coupled Receptors (GPCRs), which are the targets of about 50% of the drugs on the market. These membrane proteins mediate a plethora of critical physiological responses involved in numerous diseases. GPCRs have a paramount importance in health and disease including cancer, heart diseases, diabetes, depression and anxiety. Their very complex pharmacology remains nevertheless poorly understood.

The BioMEP group exploits state-of-the-art biophysical methods to investigate cell function. The group is furthermore specialized in exploiting novel molecules and nano-sized objects to develop novel cellular assays giving access to novel type of biological information not available today. One of the main technologies under development is based on the use of arrays of nanowires for fluorescence-based detection in live cells.

**KEYWORDS**
Membrane proteins, GPCRs, Bionanosensors, nanowires, nanoparticles, amphipols and nanodiscs, surface sensitive techniques, cellular studies.

**PEOPLE**
Associate Professor Karen L. Martinez
2 postdocs
3 PhD students

**CONTACT**
Karen L. Martinez
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Our lab is developing disruptive technologies to study the biophysical properties of membranes and membrane proteins on the nanoscale using fluorescence microscopy. Membrane proteins are one of the most important classes of proteins in biology comprising more than 60% of existing pharmaceutical targets. Biological membranes enable the function of membrane proteins and therefore play a key role in governing a plethora of biological processes. Our work uncovers hitherto unknown nanoscale properties of membrane and membrane proteins that ultimately dictate cell behavior, and consequently provides a path towards new generations of therapeutic agents based on entirely new biological principles.

The exciting problems we are investigating are situated at the interface of biology, physics and nanotechnology, and to address them experimentally we have assembled a dynamic, interdisciplinary, group of top-tier biophysicists, biochemists, molecular biologists, and nanotechnologists. Our grants and student projects are frequently in collaboration with world-leading industrial partners including Aquaporin, Chr. Hansen, Novozymes and Novo Nordisk.

Highlights from 2017

- In a breakthrough paper in Science, we demonstrated the recording of attoampere ionic currents, which allowed for the first time observation of transporter activity at the single-molecule level.
- In a breakthrough paper in Nature Chemical Biology, we demonstrated for the first time quantitative measurements of membrane curvature in live cells, which revealed that membrane curvature regulates ligand-specific membrane sorting of G protein coupled receptors.
- Professor Dimitris Stamou was elected as a member of the Editorial Board of the prestigious Biophysical Journal.
- Professor Dimitris Stamou was invited to present his work in three prestigious Gordon conferences.

KEYWORDS
Nanoscale membrane biophysics, membrane curvature, single molecules, fluorescence microscopy, Ras, G protein coupled receptors, primary and secondary active transporters.

SELECTED PUBLICATIONS
1 Kadla R. Rosholm et al., Nature Chemical Biology, 2017

PEOPLE
The group consists of approximately 15 active researchers.

CONTACT
Dimitrios Stamou
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The CECB research group combines technology and research across many scientific disciplines within a combinatorial chemistry platform. The structure of CECB provides technology for the study of complex mechanisms in molecular recognition and biochemical processing from a chemical point of view. CECB aims at understanding molecular recognition, signaling and processing. Typical topics are GPCR-signaling, enzyme and catalyst processing, molecular recognition for controlling cell behavior. The research at CECB is therefore at the interface between chemistry, biology and material sciences. CECB has developed a range of platform technologies to facilitate the study of recognition, processing and signaling. On-bead assays performed on custom-made biocompatible PEG-resins include solid-phase FRET protease substrate assays, a cells-on-bead assay for investigation of GPCR-activation, a molecular adhesion assay. Combinatorial chemistry is facilitated by optical bead encoding technology, fluorescence activated bead sorting and super high-resolution mass spectrometry.

The group CECB aims to bridge and cross-fertilize the two main personnel sub groups, one on protein chemistry, cells and chemical biology and one in organic and solid-phase combinatorial chemistry.

CECB Focus Areas
- Molecular recognition
- Organozymes, catalysis and processing
- GPCR’s
- Proteolysis
- Protein “Click” chemistry and folding
- New chemistries for targeting disease

New Chemistries
CECB has developed a reaction for the nucleophilic substitution of non-activated aryl fluorides. The reaction is used in the facile production of some important drugs currently on the market. CECB also developed complex intramolecular cascade click chemistries for synthesis of polycyclic heterocycles.

KEYWORDS
Combinatorial, Polymer, GPCR, Proteases, MS/NMR Selection, Encoding.

PEOPLE
Currently, CECB includes a total of 23 staff and students.

CONTACT
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The research group works with theoretical physics applied to a number of nanoscopic systems, quantum information systems and new materials. We collaborate and publish extensively with several world-leading experimental and theoretical research groups.

Transport through single-molecule junctions may involve interference for electrons, which transverse the junction through multiple pathways. Another interesting aspect of transport through molecules is the possibility to use their thermoelectric properties for gaining further insight and potential applications. This work is done in collaboration between physics and chemistry researchers.

This activity deals with the physical properties of the building blocks of quantum computers, which hold the information as well as ways to fabricate and manipulate these. The research has its focus on qubits encoded either in spin degrees of freedom or in topologically protected Majorana-bound states.

Unusual material properties can arise when systems exhibit strong interactions between the conduction electrons, as found, for example, in manganites, multiferroics, heavy fermions, and several families of high-Tc superconductors.

State-of-the-art experiments are currently providing new insight into the governing physics of these fascinating materials. We focus on the study of multiferroics, iron-based and copper-based superconductors using extensive numerical computations in order to extract the superconducting pairing kernel from purely repulsive interactions.

We explore the physics of new electronic phases arising at the surfaces or boundaries of topological insulators or topological superconductors. This common theme interlaces to the projects concerning quantum information systems as well as advanced materials, and has strong ties to the experimental activities within the Center for Quantum Devices.

**KEYWORDS**
Electron transport, Transistors, Superconductors, Nanowires, Molecular electronics.

**PEOPLE**
Professor Karsten Flensberg, Professor Per Hedegård
Associate Professor Jens Paaske, Associate Professor Brian Møller Andersen, Associate Professor Mark Rudner, 8 postdocs and 8 PhD students.

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The experimental research at the Niels Bohr Institute spans materials science, cleanroom nanofabrication and cryogenic measurements. In particular we focus on nanoscale electronic devices operating in the quantum regime.

The condensed matter activities comprise the Center for Quantum Devices (QDev), funded by the Danish National Research Foundation. How to create, control, measure and protect quantum coherence and entanglement in solid-state electronic devices is the main theme of the center. Specific systems investigated include devices in III-V and group-IV semiconductors and Majorana fermion systems realized in nanowires and two-dimensional electron gases coupled to superconductors.

We also investigate complex oxides and carbon-based electronics. Within the Nano-Science Center we develop nanowire-based sensors in collaboration with the Nanobioscience group, Raman imaging with NanoSpectroscopy as well as graphene and molecular electronics with NanoChemistry. We are proud of our coordinated activity in materials growth, nanoscale fabrication and electron transport measurements at millikelvin temperatures.

The group hosts a cleanroom with a suite of nanofabrication tools, including molecular beam epitaxy, scanning and transmission electron microscopes and electron beam lithography systems.

**KEYWORDS**
Condensed matter physics, nanoelectronics, quantum dots, hybrid superconducting devices, quantum bits and computing, quantum coherence, topological systems, Majorana fermions, nanowires, nanotubes, epitaxial semiconductor growth (MBE), complex oxides, electron microscopy (TEM), sensors

**PEOPLE**
2 professors, 3 associate professors, 4 assistant professors, 8 postdocs, 15 PhD students, 10 MSc students

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Experimental NanoElectrocatalysis

Our research group investigates novel electrochemical interfaces for sustainable energy conversion devices (e.g. fuel cells and electrolysers) and electrocatalytic synthesis of chemicals. We combine electrochemical methods with surface science characterisation, in-situ optical spectroscopy, microscopy, gas chromatography-mass spectrometry and in-situ synchrotron-based X-ray characterisation techniques in order to understand the structure of the electrochemical interface at the atomic and molecular level. We carry out model studies aiming to understand and tune the activity and selectivity of different electrochemical reactions as well as solving the fundamental challenges that impede the large scale uptake of electrochemical energy conversion technologies. We work in close collaboration with theoretical and experimental groups both at UCPH and international groups at Stanford University, the University of California Berkeley and Massachusetts Institute of Technology, as well as large companies including Haldor Topsøe.

Highlights from 2017
- DKK 10 million VILLUM Young Investigator Grant awarded to María Escudero Escribano.
- The Royal Society of Chemistry (RSC) awarded María Escudero Escribano with the prestigious Griess Lectureship 2017.
- María Escudero Escribano was honoured to be elected as a Board Member of the Danish Electrochemical Society.
- Awards received: María Escudero Escribano received the CIDETEC Award for Young Researchers in Electrochemistry by the Electrochemistry Group of the Spanish Royal Society of Chemistry and the SUSCHEM Young Chemistry Researcher Award by the Spanish Royal Society of Chemistry.

KEYWORDS
Electrochemistry, Electrocatalysis, Nanomaterials, Surface Chemistry, Sustainable Energy Conversion, Electrochemical Synthesis

SELECTED PUBLICATIONS

PEOPLE
Assistant Professor María Escudero Escribano
Postdocs: Kim D. Jensen, Jonathan Quinson
PhD students: Anders W. Jensen, Bethan J.V. Davies
MSc students: José Alejandro Arminio-Ravelo, Hannibal M. Schultz

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Our research lies at the intersection between chemistry and nanoscience. We build and study electronic devices that employ organic molecules as a key functional component. The aim is to understand the nature of electrical conductance properties of organic molecules when integrated in permanent solid-state nanodevices.

Additionally, we synthesize 2D nanomaterials (graphene) and metallic nanostructures that can be used in e.g. nanoelectronics or as additives in coatings or composites, where they provide new remarkable properties to the material.

Recent projects:

- Molecular vibrations and charge transport studied at ultralow temperatures in solid-state devices.
- Development of antistatic and anti-corrosive coatings based on graphene-polymer composites.
- Highly conducting and semi-transparent graphene inks for printing.
- Carbonhagen 2017 – symposium on graphene and 2D materials.

**KEYWORDS**
Molecular electronics, graphene materials and composites, self-assembly, surface chemistry.

**PUBLICATIONS**

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We are two theoretical groups in the Department of Chemistry studying charge and energy transport through molecules. We are interested in conducting junctions, solar cells and photosynthetic protein complexes.

Highlights from 2017
The Solomon group’s activities were focused around our major project “Simulating Single-Molecule Pulling Experiments” under a Sapere Aude grant. In 2017, four PhD students and two postdocs have been working on the project and we have had a number of exciting results. Our efforts resulted in 10 peer-reviewed publications for 2017. As this project draws to a close in early 2018, we have had four PhDs complete their theses in 2017.

GCS has also continued to work as a Senior Editor for the Journal of Physical Chemistry A/B/C.

The Hansen group focuses on its major project “Charge Transfer and Catalysis in Metalloproteins” funded by the Lundbeck Foundation. The first PhD graduated from the group in October 2017. We congratulate former group members Luca De Vico, now assistant professor in Siena, Italy, and André Anda, now postdoc in Melbourne, Australia.

**KEYWORDS**
Molecular electronics; charge transfer and transport; quantum interference; inelastic electron tunneling spectroscopy; energy transfer; coherent multi-dimensional spectroscopy.

**PEOPLE**
Gemma C. Solomon  
Thorsten Hansen  
1 Postdoc  
4 PhD students  
1 PhD student  
2 MSc students

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The Molecular Engineering Group seeks to design, synthesize, and study functional macromolecules, in particular π-conjugated molecules. All activities are rooted in organic synthesis. Within the Center for Exploitation of Solar Energy (www.ki.ku.dk/Forskning/cese/), a special emphasis is on development of new organic molecules for energy storage and photovoltaic. Other important activities are development of redox-active organic molecules for molecular electronics, photoswitchable liquid crystals, and two-dimensional redox-active carbon-rich sheets and networks.

Highlights from 2017
Significant progress with respect to controlling the switching cycles of dihydroazulene/vinylheptafulvene photo-/thermoswitches has been achieved. This control is particularly important in the quest for light-harvesting molecules for solar energy storage, that is, molecules that harvest solar energy by undergoing a photoisomerization reaction and release the energy again as heat on demand when needed. We have also developed and synthesized several new functional organic molecules for molecular electronics applications, including new cruciform motifs based on redoxactive tetrathiafulvalene and dithiafulvalene units.
Our research is focused on the interface between synthetic bioorganic chemistry, biology, biophysics, medicinal chemistry, and nanotechnology. We are in the section for chemical biology at the Department of Chemistry.

We seek to define and exploit the laws governing self-assembly of biomolecules in order to build biological meaningful nano-scale structures. The aim is to understand and control the self-assembly of biomolecules in solution and on surfaces. The ability to make defined nano-scale structures of biomolecules leads directly to biomedical applications, including nanomedicine.

Organic synthesis is a powerful tool for the design and preparation of new materials on the Ångström and nanometer-length scale. We use a combination of solution and solid-phase based organic chemistry to synthesize complex biomolecules, such as peptides, glyco-conjugates (carbohydrates), and even small proteins. We also develop new chemistry, including new reagents, to aid us in the synthesis of complex biomolecules. For example, we are working with designer proteins, which are man-made protein-like molecules with an artificial structure, which we are using in studies on self-assembly, both in solution and as self-assembled monolayers on surfaces.

To study these structures, we collaborate with biophysicist and physical chemists. We are using the knowledge gained in these studies in collaboration with partners from the biopharmaceutical industry.

In one line of research, we are anchoring abiotic ligands covalently and regioselectively to proteins to control their self-assembly at the nano scale. We have shown that non-native bipyridine ligands can be used to control the higher-ordered self-assembly of insulin.

The use of Fe(II) provided chemoselective binding over the native site, forming a homo-trimer in a reversible manner, which was easily followed by the characteristic color of the Fe(II) complex. This provided the first well-defined insulin 18-mer and the first insulin variant where self-assembly can be followed visually.

**KEYWORDS**
Nanobioscience, medicinal chemistry, nanoparticles, surface chemistry, chemical synthesis, peptides, protein, carbohydrates

**SELECTED PUBLICATIONS**
1 C. Lou et al, Nature Communications, 2016, 7:12294

**PEOPLE**
Mikkel B. Thygesen, associate professor, Knud J. Jensen, professor

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In the Nano Chemistry Group our research focuses on the interaction between light and molecules. We use the fundamental insight on these processes to design and synthesize materials and molecules that can act as fluorescent stains and probes to detect and visualize nanoscale structure and processes.

Our main tools are design and synthesis of new organic and f-block containing molecules and materials with new or improved optical properties.

Recent projects:

- Development of intensity ratiometric oxygen probe based on lanthanides.
- Development of anti-counterfeiting materials based on nanoparticle imaging.
- New of high contrast cell stains based on time gated fluorescence.
- Improved fluorescent pH indicators.

**KEYWORDS**

Fluorescent dyes and sensors, Organic synthesis, Lanthanides, fluorescence imaging, Time resolved fluorescence.

**PUBLICATIONS**


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The primary focus of our lab is to provide the molecular level mechanisms that underlie and control protein behavior with special emphasis on structure function correlations and biomolecular interactions. Harnessing this knowledge is the founding step to tackle the daunting tasks of a) design novel drugs in silico for improving human health and b) the design of novel biocatalysts with tailor-made functionalities for biotechnological green energy solutions.

Single-molecule studies (functional, FRET particle tracking), offer the grave potential to directly observe the existence, quantify the abundance and dependence on mutations, of behaviors that were masked in conventional assays due to averaging a large number of unsynchronized molecules. Interrogating the structural and functional dynamics of an enzyme allows us to provide links between nanometer motions and ultrafast structural dynamics to human diseases and industrial performance (e.g. detergent pharmaceutical industry).

All our projects are in tight collaboration with industrial partners (e.g. Novozymes, Novo Nordisk), medical doctors, and biological labs and are at the interface between chemistry, biology, biophysic, medicine and clinical biochemistry.

News in 2017
In the last years Nikos S Hatzakis got awarded the Young Investigator fellowship by Villum and Distinguished Associate Professor fellowships by Carlsberg, that is directed to especially talented up-and-coming researchers in science and technology with ambitions of creating and expanding their own independent research groups, respectively. Combined with recent grants from Lundbaek foundation, Marie Curie fellowship as well as Velux center of excellence “BIONEC” allowed the lab to be fully equipped with state-of-the-art super-resolution single-molecule microscopes while we are hiring new members.

SELECTED PUBLICATIONS

PEOPLE
Postdoc: Min Zhang Pradeep K Singh, Condruta Ignea
PhD students: Matias Moses, Simon Bo Jensen, Johannes Thomsen, Søren Rasmussen, Camilla Thorlaksen
MSc Students: Mette Gaalsgard Jullie Dihtmar Darui Li, Amalie Kallenbach, Phillip Mark Lund

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We are a young group at the Nanoscience Center and at UCPH, studying the synthesis and atomic structure in nanomaterials for energy conversion and storage. By means of advanced scattering techniques, we look into the arrangements of atoms in smart materials in an effort to map the relation between structure, synthesis and properties.

Nanomaterials by design

In order to get to the next stage of nanomaterial technology, where advanced nanomaterials can be ‘designed’ to have specific properties needed for advancing energy applications, it is crucial to understand the atomic structure on the nanoscale. Structural understanding of nanomaterials is exactly the focus of our research. By means of high-energy synchrotron X-ray radiation, we work on elucidating the structure of complex nanomaterials. We go beyond traditional crystallographic methods for structure analysis, allowing us to determine the atomic arrangements in nanomaterials. We are also able to follow material synthesis in situ to get a glimpse of nanostructure formation and elucidating fundamental reaction mechanisms in nanochemistry. We study a broad range of energy materials, with applications in solar cells, batteries, catalysis.

We are frequent users of synchrotron and neutron facilities in Europe and the US, we are part of the development of new methods for nanostructure characterization.

Highlights of 2017

Kirsten recived the Villum Young Investigator grant from the Villum Foundation (10 million DKK) to build up a strong, leading group in materials characterization. She furthermore recived the L’Oreal UNESCO For Women in Science Award.

KEYWORDS


SELECTED PUBLICATIONS

1 Espen D. Bøjesen et al Chemical Science 7 (10), 6394-6406, 2016
3 Kirsten M. Ø. Jensen et al Nature Communications, 7, 11859, 2016

PEOPLE

Kirsten M. Ø. Jensen, 1 PhD student, 5 master students, 2 bachelor students.

CONTACT

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Nanotechniques let us “see” at the nanometre scale, where all the action is. We use them to learn nature’s secrets, to understand the fundamental physical and chemical processes that take place at the interface between natural materials and fluids (water, oil, CO₂, O₂, anything that flows). Then we use our new knowledge to find solutions to society’s challenges.

The challenges we tackle include finding ways i) to ensure safe drinking water, ii) to store waste responsibly, iii) to convert CO₂ back to rock form where it will be stable for thousands of years, iv) to understand how organisms make biominerals, such as bones, teeth and shells and v) to squeeze a bit more oil from reservoirs that are reaching the end of their lifetime. Our research on how organic compounds interact with mineral surfaces also provides better insight into how to remediate contaminated drinking water aquifers, and offers clues for how fluids flow in other porous media such as catalysts, filtration systems, soils and sediments. Our approach is well suited for characterising natural nanoparticles in general, such as the volcanic ash that closed Europe’s airspace. Occasionally we contribute information and data interpretation for the Mars mission.

The NanoGeoScience group works closely with X-ray Physics in the Nano-Science Center and has tight partnerships with the Physics Department at DTU (Danish Technical University) and universities in Toulouse, F, Leeds, Warwick, University College London, York, Sheffield and Cambridge, UK; Oslo, N; Reykjavik, I; Karlsruhe, Münster and Potsdam, D; Waterloo, Canada; Berkeley and PNNL, USA as well as with several companies, including Maersk Oil, BP, Reykjavik Energy, Rockwool, Haldor Topsøe, Níras, COWI, GEO, Amphos21, AE-COM and Arcadis.

**KEYWORDS**
Natural materials, surface chemistry & physics, solid-fluid interface, water quality, safe waste disposal, CO₂ sequestration, enhanced oil recovery (EOR), biomineralisation, volcanic ash characterisation, nanometre scale characterisation techniques, interdisciplinary, industry-university partnership.

**SELECTED PUBLICATIONS**

**PEOPLE**
Profs S. Stipp (Section Leader) and K. Bechgaard, Assoc. Profs H.O. Sørensen, D.J. Tobler, N. Bovet, M.P. Andersson, T. Hassenkam, K.N. Dalby, L. Lakshtanov; 4 Ass. Profs; 6 Re-search, Technical and Admin. Associates and Assistants; 12 Postdoctoral Fellows; 15 PhD, several Master and Bachelor Students; 2 Guest Researchers.

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Hanne Mørck Nielsen, Vito Foderà and Marco van de Weert are from the “Drug Delivery and Biophysics of Biopharmaceuticals” group at the Department of Pharmacy, UCPH. The “Center for Biopharmaceuticals and Biobarriers in Drug Delivery” is embedded within the group.

The group seeks to exploit the extraordinary structural and functional properties of peptides and proteins within various pharmaceutical applications. More specifically, our research can be divided into two main areas.

In the first area we aim at developing experimental and theoretical platforms to understand and control the protein and peptide self-assembly process at the single-molecule level. This knowledge is pivotal for the design of effective treatments for protein-related pathologies as Alzheimer’s and Parkinson’s disease, increasing the stability of protein drugs and developing reliable bottom-up approaches for protein biomaterials growth. To this aim we combine various spectroscopic and calorimetric methods with advanced analysis of X-ray and Neutron scattering data and imaging. Theoretical models are also developed for the quantitative analysis of the experimental data.

The second area focuses on the interplay between macromolecular therapeutics and biological barriers in order to advance the design of drug delivery systems for therapy with peptide and protein drugs. We take a mechanistic approach to understanding the detailed interplay between the drug molecules, the excipients, the drug delivery systems, and the biobarriers seen in a global perspective. Through formulation design, including modification of the peptides and proteins and use of advanced delivery systems, we aim to improve the delivery of these potent therapeutics into and across biobarriers.

**KEYWORDS**
Amyloid-like Aggregation, Protein-Membrane Interactions; Protein aggregation; Protein Stability; Theoretical Models for Self-Assembly; Spectroscopy; Transmission Electron Microscopy; X-ray Scattering Membrane-interacting Peptides, Biopolymers, Nano- and Micron-sized Drug Delivery Systems, Membrane Interaction, Uptake and Transport, Mucus Interactions, Cell Culture Models, Cell Toxicity

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Our research group has a strong focus on studying the fluorescence properties of individual fluorophores by combining spectroscopy with microscopy. Single-molecule spectroscopy is a multidisciplinary technique, which has found many applications in the field of material and life science characterization. A large variety of topics have benefitted from the advent of single molecule spectroscopy and yielded fundamentally new insights. Additionally, recent developments allow for fluorescence imaging beyond the diffraction limit, opening up a new dimension in microscopy. Our group studies the photophysical properties of organic fluorophores at the single molecule level and we also develop new fluorophores (silver nanoclusters) for single-molecule spectroscopy applications. Beside fluorescence we are also interested in studying Raman and SERS from nanoscale materials, the latter in collaborations with other research groups. We currently we have a piezo-scanning confocal microscope that is coupled to 2 APDs and an EMCCD-based spectrometer. This allows us to do single-molecule fluorescence spectroscopy (simultaneous recording of fluorescence intensity, fluorescence decay time, emission spectra, polarization or antibunching), micro-Raman spectroscopy, Raman imaging or SERS.

As excitation sources we have a whole range of CW and pulsed lasers that allow us to excite samples from the UV to near-infrared. Besides a confocal setup, we also have two wide-field setups. One of these setups is designed for use as a high-resolution fluorescence localization microscope (e.g. STORM, PALM-like imaging). Time-correlated single photon counting, FCS, FLIM and antibunching can be performed by our Becker & Hickl SPC-830 card. Highlights include 9 new research papers on topics like characterization of dyes, single molecule spectroscopy, micro-Raman and silver nanoclusters.

**KEYWORDS**
Single molecule fluorescence spectroscopy, micro-Raman spectroscopy, steady-state and time-resolved fluorescence spectroscopy, silver nanocluster fluorescence.

**SELECTED PUBLICATIONS**

**PEOPLE**
The group currently counts 1 Associate professor, 2 PhDs and 2 postdocs

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Our focus areas include adverse health effects of particles from air pollution both outdoors and indoors and engineered nanoparticles and nanomedicine, as well as the involved mechanisms of action in particular related to oxidative stress and vascular functions.

The section carries out basic research on environment and health throughout the life course, with methods ranging from experimental models to register-based epidemiology. The priority of the section is to contribute to future public health and prevention with original research and training of talented researchers.

The work spans the entire hierarchy of methods from experimental models such as synthetic membranes, organotypical cell co-cultures with advanced optical instruments and transgenic animals, through the use of biomarkers and functional goals in populations with controlled exposure and interventions in particularly sensitive groups, to register-based epidemiology at the aggregate level.
The research of the Organic Materials and Catalysis Group tackles current global issues such as CO₂ emission, CO₂ functionalization and desalination by applying organic and organometallic materials in catalytic processes. By taking advantage of the knowledge in organic synthesis, heterogeneous catalysis and asymmetric catalysis, we will provide ground-breaking methodologies to provide solutions in chemical, environmental, and pharmaceutical sciences.

Catalysts promote desired chemical transformations at lower energy expenses than non-catalyzed reaction; ideally, they do so for an infinite number of cycles, by in-situ regeneration of the active catalytic species without alteration of its molecular structure or physicochemical properties. To mitigate the ever-growing CO₂ concentration in the atmosphere, the group’s research is focused on catalytic conversion of carbon dioxide to useful synthetic building blocks. This work implies that industrial waste, namely CO₂ can be transformed to industrially useful chemicals, serving as a fuel source.

The group’s research also covers a broad range of areas in organic chemistry and material chemistry, aiming at industrial applications by providing new catalytically active homogeneous and heterogeneous organic- and organometallic materials and water purification technologies. The obtained functionalized organic materials will be also applied in biological processes, particularly to capture heavy metal ions related to Alzheimer’s and Parkinson’s diseases.

**KEYWORDS**
Carbin Dioxide, Desalination, Organic synthesis, Catalysis, Chirality

**SELECTED PUBLICATIONS**
2 Ji-Woong Lee et al., Chem. Soc. Rev. 2016, 45, 4638-4650.
3 T. Mayer-Gall et al., ChemCatChem 2016, 8, 1428-1436.

**PEOPLE**
Assistant Professor. Jee-Woong Lee, 1 PhD student, 2 MSc students, 1 Research Assistant

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The vision with the research is to develop electrocatalysis for production of sustainable fuels and chemicals. The properties of the electrochemical devices are often related to the atomic structure of the interfaces. Atomic scale insight is needed to fundamentally understand and eventually improve the interfaces. We apply density functional theory (DFT) computer simulations to study the interfaces as DFT in this case is the electronic structure method that offers the best trade-off between accuracy and system size. We work in close collaboration with international experimental groups, large companies: BMW, Topsøe, Covestro and startup companies: HPNow and Hymeth.

Highlights from 2017:

- Proactive project was stated in March. It is a grand solution project from Innovation fond Denmark in collaboration with Topsøe A/S, HP Now APS, DTU and Stockholm University.
- The Villum Center for the Science of Sustain-able Fuels and Chemicals was started in August. We are heading one of the subprojects, it will run over the next 8 years.
- PhDs: Martin Hangaard, Michael Fleige and Yu jia Deng graduated.

KEYWORDS
Sustainable Chemistry, Catalysis, Electrocatalysis, Electrochemical Interfaces, Energy Conversion, Electrochemical Production of Chemical, Batteries, Atomic Scale Simulations.

SELECTED PUBLICATIONS
1 Hansen, Martin H.; et al. SCIENCE, 352, 73-76, 2016
3 Kramm, Ulrike I.; et al. NANO ENERGY 29, 126-135, 2016
4 Rossmeisl, Jan et al. CHEM CATCHEM 8, 3334-3337, 2016
5 Hodgson, Andrew et al. CHEMICAL REVIEWS 116, 7698-7726, 2016

PEOPLE
Postdoc: Ivano Castelli, Manuel Saric, Logi Arnarson.
PhD students: Luca Silvioli Thomas Østergaard, Alexander Bagger, Bethan Davies, Søren Bertelsen Scott, Kaspar Holt-Olesen, Anders Holten
MSc students: Hao Wan, Ahmad Balal Gardizi, Hannibal Morten Schultz, Anderas Swane, Marta Roqulle

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The X-ray and Neutron Science Section focuses on structural materials sciences in a broad scope, ranging from magnetism and superconductivity to synthetic polymers, bio-molecules and pharmaceutics. The X-ray and Neutron Science Section is further involved in the design and development of new instrumentation for large scale international facilities, and for the development of new numerical tools for analyzing and predicting properties of such new instruments as well as properties of new materials. Specific materials properties that are studied both experimentally and theoretically include quantum phase transitions and the interplay between magnetism and superconductivity. Inelastic neutron scattering methods is applied to study hydrogen dynamics as well as the nanoscale hydrogen bonded network, which is a key parameter in many new green-materials. Polymers and colloids typically respond with a large effect when exposed to even very small stresses and shear forces. Understanding the related structure-function relationship is crucial for the design and development of new materials. A large effort is made in the context of synthetic biology to make new artificial bio-based materials. The concept of nano-disk is particular central for structural investigations of membrane proteins.

**KEYWORDS**
Sustainable Chemistry, Catalysis, Electrocatalysis, Electrochemical Interfaces, Energy Conversion, Electrochemical Production of Chemical, Batteries, Atomic Scale Simulations.

**SELECTED PUBLICATIONS**
2. K Mortensen and M Annaka. ACS MacroLet 5, 224, 2016
3. ML Martins et al. SCI REPORTS 6, 22478m 2016

**PEOPLE**
Kell Mortensen, Robert Feidenhans'l, Lise Arleth, Brian Vinter, Stig Skelboe, Kim Lefmann, Brian Møller Andersen, Heloisa N. Bordallo, Lars H. Øgendal, Steen L Hansen, Linda Udy and Jacob Kirkensgaard. 6 postdocs and 25 PhD students.

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