Frontcover
Lab-on-a-chip by Liridon Aliti, Martinez Group, Nano-Science Center, University of Copenhagen.

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”Sunflower party” by Benoît Desbiolles & Valentin Flauraud, Center of MicroNanoTechnology, EPFL; ”A man facing a wall” by Benoît Desbiolles, Center of MicroNanoTechnology, EPFL; ”Towering Chalk” by Anton Bischoff, NanoGeoScience, Nano-Science Center, University of Copenhagen; ”Mineral cauliflowers” by Juan Diego Rodriguez Blanco, Trinity College Dublin, Dublin · Department of Geology;

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Coloured tight junctions in Caco-2 cells by Martin Roursgaard, Nanotoxicology – Particles & Oxidative stress, Nano-Science Center, University of Copenhagen.

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”Fluorescent DNA” by Liridon Aliti, Martinez Group, Nano-Science Center, University of Copenhagen.

Back cover
”Demonstration of topological quantum computation via nanowire device” by Davydas Razmadze, Center for Quantum Devices, Nano-Science Center, University of Copenhagen.
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Nano-Science Center

The Nano-Science Center with the University of Copenhagen is one of 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 NSC each bring in high-level expertise in various areas of theory, experimental methods and instrumentation into joint research projects and into the nanoscience 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 13 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.
2016 in short

Highlights of the Nano-Science Center activities include:

- The nanoscience undergraduate programme enrolled 50 students in September, and 36 students joined the Master’s programme in nanoscience.

- The Sino-Danish Center for Education and Research (SDC) continued their Master of Science programme in Nanoscience and Technology in Beijing. The programme is organized jointly by the Nano-Science Center and iNANO at Aarhus University.

- A total of 12 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 7th international symposium Carbonhagen together with DTU Nanotech and reached a total of 160 participants in 2016.

- Attracting new researchers:

  Three new research groups have become members of the Nano-Science Center:
  Professor Peter Møller and Associate Professor Martin Roursgaard became members with their group Particles and Oxidative Stress, Department of Public Health, Faculty of Health and Medical Sciences, University of Copenhagen

  New tenure-track Assistant Professor Jiwoong Lee was recruited from University of California, Berkeley, USA to form the new group in Organic Synthesis and Catalysis.

  Professor Hanne Mørck Nielsen, research head of the group in Peptide and Protein Drug Delivery, became a member together with Associate Professor Marco van der Weert and Associate Professor Vito Foderá from the group Protein Formulation and Biophysics, section for Biologics, Department of Pharmacy, Faculty of Health and Medical Sciences, University of Copenhagen.

Happy reading
Bo Wegge Laursen and Tine Buskjær Nielsen
The new student journal, UCPH Nanoscience, is a unique way to publish student articles, and most of the nanoscience bachelor projects will be published here in the future along with articles from courses or research internships.

The editor-in-chief, Associate Professor Thomas Just Sørensen, was satisfied when he spoke to the students at the launch of the student research journal:

“It’s a journal with student editors and the authors are students, but the readers are both local researchers and scientists around the world. Some call the journal a kind of a yearbook, where you can follow the work of your fellow students. But it is more than that, when also the researchers read your articles, it’s an opportunity.

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

You may find the journal at tidsskrift.dk

If you would like a copy of the journal, please contact Tine Buskjær Nielsen at tinebuskjaer@nano.ku.dk.
Every year, about 65,000 students start a higher education programme in Denmark, and every year stories from the introduction weeks are in the news, most often stories about too much booze or parties gotten out of hand. This year, the story of the week was the positive story about nanoscience at University of Copenhagen in the daily newspaper Information.

The total of 50 nanoscience freshmen and their tutors met with freshmen from other parts of UCPH and were welcomed by rector. Up to this, the tutors had spent the last month planning the introduction week. The nanoscience introduction programme includes a number of name games, where you tell which pizza describes you best or describe why you chose to study nanoscience. In 2016, the students had been sought out by an unexpected journalist. After several years with horror news each August, the story about nanoscience broke free from previous years. A few days later, Information published the positive story about the introduction week here at nanoscience.

Overall, the introduction week on our BSc degree programme in nanoscience was an incredible success, where the first-year students were integrated into the “nano” community. Moreover, it was a pleasure that Information was there to witness it.

Find the article here: http://bit.do/Nanointro
ARTiS - Art in Science

The ARTiS competition 2015 was the first time a competition of this kind took place at Faculty of Science. Again this year, ARTiS was a great success with hundreds of photos, a well-organized contest and broad interest during Culture Night in Copenhagen!

To be a researcher is about being the best on a specific field, knowing the methods, the theory, designing experiments and doing the calculations. You have to be clever, smart and creative. All along, we educate ourselves to do better, we never stop learning, and we wish to be the best on our field. But sometimes we forget that to be a great researcher, we also need to be creative. It is important to be innovative and rethink problems if we want to solve them. That is what ARTiS is all about!

ARTiS, Art in Science is an art competition about the creative side of science, it is a contest with room for everybody from highschool pupils to well-known scientists, all with that in common that focus is the creative side of research, which put them all on same level. The pictures have to be of science, but they are judged on the art. The event is sponsored by Lundbeckfonden and University of Copenhagen and organized by Karen Martinez, associate professor, Nano-Science Center.

One of the beautiful pictures this year was from the Danish-French school, who won the Young ART-scientist award to a fun day with the ARTiS team in the lab playing with green fluorescent protein, cells and bacteria. It is the picture in the middle to the right.
A year full of prices!

The year 2016 was full of acknowledgement to researchers in the Nano-Science Center: Villum Grant, Torkil Holm Research Award, new member of the young academy, the Innovation Price and Novo Nordisk Grant.

Villum Foundation
Two young researchers at the Nano-Science Center have received DKK 10 million each to understand relations between structure and function on the nanoscale. Where Assistant Professor Kirsten M. Ø. Jensen's research can lead to new nanomaterials that can improve technology for energy conversion and storage, Associate Professor Thomas Just Sørensen's work will attempt to secure access to the raw materials that this type of high-tech applications consume. The two research projects, which Villum Foundation's Young Investigator Programme supports, both have a large element of fundamental research and focus on increasing our understanding of how the world works. In future, the basic scientific discoveries may form the basis of new technologies.

Torkil Holm Prize:
All actions of living beings start with molecules interacting. But figuring out which molecules go where when we get sick, get well or fall in love is a formidable challenge. One of the few who can rise up to it is Dimitrios Stamou. He is professor of chemical biology at the Nano-Science Center. Dimitrios Stamou is a leading expert in the physical chemistry of biological systems and works on uncovering the chemical mechanisms underpinning biological processes. He is also developing methods to control and study chemical reactions at the single molecule level. He is a prolific author of scientific publications with, among others, four publications in Nature periodicals and one in Science to his name. Now he is awarded the highly prestigious Torkil Holm prize for his work on the borders between chemistry and biology, which consist of DKK 50,000.
UCPH Innovation Price 2016

The 2016 Innovation Prize was awarded to two researchers at the Nano-Science Center, whose spin-out projects have raised millions in venture capital, established collaboration with Danish industry heavyweights and involved students in the journey from basic research to the sale of optical sensors and dyes. Associate Professor Thomas Just Sørensen and Professor Bo Wegge Laursen have involved both BSc, MSc and PhD students in innovation from basic research to solid business plans. They have started two spin-outs, raised venture capital and now have specific products and a large network of business partners in industry, as well as motivating and engaging the students in their research.

New member of the Young Academy

Thomas Just Sørensen has become a member of the Young Academy, with the purpose of strengthening career and development of young investigators. Also, the Young Academy unites science and community, which gives the members a public vote. With Thomas as member of the Young Academy, the programme in nanoscience has a new spearhead, a committed teacher and talented researcher working to promote agendas.

Novo Nordisk Foundation Challenge Programme:

New member of Nano-Science Center, Professor Hanne Mørck Nielsen has been granted DKK 60 million from the Novo Nordisk Foundation Challenge Programme, of which Professor Knud Jørgen Jensen has been granted DKK 12 million. Aimed at leading researchers, the Foundation Programme awards grants of DKK 60 million over 6 years to research groups, thereby enabling them to have the funds to carry out in-depth research on a specific theme over a long time frame.

"This major project involves advanced chemistry, nanorobots and visualizing the transport of drugs in the body. This will enable us to design and study systems for oral drug delivery of biopharmaceuticals."

Hanne Mørck Nielsen
Professor and member of the Nano-Science Center.
Publications & Citations

In 2016, researchers from the Nano-Science Center successfully published more than 145 peer-reviewed papers. Their works were cited more than 11,500 times.
New members of the Nano-Science Center

With three new research groups joining the Nano-Science Center in 2016, the Center becomes an even broader network which offers cooperation across faculties.

Jiwoong Lee
Jiwoong Lee has already impressed the Nano-Science Center with his communication skills and good sense of humour at his seminar in November 2016, where some of his points were made more understandable with references to Pikachu and the rest of the Pokémon world. Jiwoong presented his group’s goal as developing new catalytic methodologies for organic synthesis. With state-of-the-art functionalised materials, they will convert CO$_2$ into useful chemicals suitable as fuel.

Martin Roursgaard and Peter Møller
From the Department of Public Health at the Faculty of Health and Medical Sciences, Martin Roursgaard and Peter Møller are new members of the Nano-Science Center with their group in Particles and Oxidative Stress. They are investigating in a broader understanding of the environment and health through life. Especially research in the effects of particles from air pollution, engineered nanoparticles and nanomedicine is carried out. The methods are varied from experimental models to register-based epidemiology at the aggregate level.

Hanne Mørck Nielsen, Marco van der Weert and Vito Foderá
From the Department of Pharmacy at the Faculty of Health and Medical Sciences, Hanne Mørck Nielsen, Marco van der Weert and Vito Foderá are new members of Nano-Science Center. The group focuses on design, development and characterization of drug-delivery systems using efficient and safe drug carriers as lipids or polymers. Often the targets are intracellular, which makes nanosized drug delivery systems a solution in order to penetrate membranes.

In 2016, Hanne received DKK 60 million from the Novo Nordisk Foundation Challenge Programme to further investigation of new unique drug-delivery concepts, technologies and methods.
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 NSC 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 class.

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

Science Dating
Where students meet representatives from industry. Twelve 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 2016, the research groups in the Nano-Science Center received funding from national and international funding agencies and private foundations.

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 2016:

Maersk Olie og Gas
BP
DONG Energy
Reykjavik Energy
Rockwool
Haldor Topsøe

Niras
COWL
GEO
Applied Biomimetic
BMW
Novo Nordisk

Gubra aps
Novartis
Quantumwise
Hempel
Medtronic
Novozymes
Graduated PhDs in 2016

Vivien Jagalski
"Molecular interactions at membranes: Examples of a biomembrane reconstitution on a surface and diterpene-lipid interactiones."

Yujia Deng
"Systematic investigations of the oxygen reduction reaction on Pt based catalysts comparing transient and steady state performance."

Samuel McEwen Walsh
"High content analysis methods to study PCR oligomerization."

Michael Josef Fleige
"High Temperature Polymer Electrolyte Fuel Cells - Development and application of experimental catalyst investigation tools."

Klaus Villadsen
"Bio-conjugates for Nanoscale Applications."

Reza Gooya
"Improved Insight into Transport Phenomena in Porous Materials at Submicrometer Resolution."

Freja Chabert Østerstrøm
"Atmospheric Gas-Phase Reactions of Fluorinated Compounds and Alkenes."

Mario Ficker
"Dendrimer Phthalocyanine Theranostics for Fluorescence Imaging and Photodynamic Therapy of Atheromatous Plaques of Atheromatous Plaques."

Bi Yun Zhen Wu
"A combined thermodynamic and kinetic model for barite prediction at oil reservoir conditions."

Surendra Vutti
"Covalent Organic - Metaloxide Modification of Nanostructure Surfaces for Protein and Intracellular Interaction Studies."

Xintai Wang
"Molecular Electronics of Self-Assembled Monolayers."

Diwaker Jha
"Improved Flow Property Determination from Nanotomography of Porous Media."

Nina Buch-Månson
"Exploring nanostructure arrays for single-cell and subcellular manipulation and detection."

Kim Jantzen
"Endothelial progenitor cells, leucocyte mediate production of reactive oxygen species and exposure to indoor and outdoor air pollution."

Josefine Frida M S Kornerup
"Paediatric photon and proton radiotherapy treatment planning based on advanced imaging."

Anna Fedrigo
"Neutron Instrumentation and Neutron Investigation of Archaeometallurgical Arms and Armours."

Sven Marian Albrecht
"Quasiparticle dynamics and Exponential Protection in Majorana Islands."

Tomas Stankevic
"Structural investigations of semiconductor nanowires."

Vladimir Posvyanskiy
"Quantum and Classical Approaches in Graphene and Topological Insulators."

Mikkel Schou Nielsen
"Applications of novel X-ray phase-contrast imaging modalities in food science."

Maria Navarro Gastiasoro
"Emergent disorder phenomena in correlated Fe-based supercunductors."

William Hvidtfelt Padkær Nielsen
"Quantum Cavity Optomechanics with Phononic Bandgap Shielded Silicon Nitride Membranes."

Henrik Jacobsen
"Complex magnetic systems studied with neutron scattering."

Morten Sales
"Development of Instrumentation for Spin-Echo Induced Spatial Beam Modulations for Small Angle Scattering Investigations."

Jakob Meyer-Holdt
"Experimental methods for implementing graphene contacts to finite bandgap semiconductors."

Sonja Lindahl Holm
"Neutron scattering investigations of correlated electron systems and neutron instrumentation."

Anders Robert Jellinggaard
"Quantum Dots Coupled to a Superconductor - Theory and Experiments based on InAs Nanowires."

Daniel Vest Christophersen
"Mechanisms of accelerated atherosclerosis by exposure to carbon-based nanomaterials."

Jerome Thomas Mlack
"Growth and Low Temperature Transport Measurements of Pure and Doped Bismuth Selenide."
Research groups
The group exploits novel nanotechnologies and bio-physical techniques for the investigation of G protein coupled receptors (GPCRs), which are the largest protein family in the human genome and mediating a plethora of critical physiological responses involved in numerous diseases. Despite the paramount importance of GPCRs in health and disease, their pharmacology remains one of the most complex and less understood. We follow two complementary strategies to investigate GPCRs at the nanoscale: (i) in living cells using quantitative fluorescence microscopy and (ii) as isolated systems immobilized onto surfaces. We also exploit novel nanomaterials and in particular high-aspect-ratio nanostructures for the development of: (i) in cell biosensors suitable for the fundamental investigation of membrane protein signaling and the establishment of novel generation of cellular assays for drug discovery; (ii) 2D and 3D protein arrays suitable for bioanalytics, proteomics and diagnostics.
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 themselves 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.

**Highlights from 2016**

- 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.

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.

**KEYWORDS**

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

**SELECTED PUBLICATIONS**


**PEOPLE**

The group consists of approximately 15 active researchers.

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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 is currently 23 coworkers and students. We are working in areas that range from cells to development of new organic reactions, and the group consists of researchers with a great variety of expertise. CECB aims to bridge and cross-fertilize the two main personnel subgroups, 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

CECB has developed a platform for expression YFP upon GPCR activation
Molecular bead-bead interaction assays were used to identify small molecules displaying specific electrostatic recognition in water. We developed a range of substrate specific catalysts that hydrolyze peptide bonds. These metallo-peptides were also promising as region-selective catalysts for organic transformations such as Suzuki reactions.

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.

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At CECB we make combinatorial libraries of metal binding peptides that show activity in peptide hydrolysis.
Understanding electronic properties of nanoscopic objects requires a joint scientific effort combining several scientific approaches, such as chemical and physical experiments and theories. Experiments can give rise to questions that cannot be described within the established theoretical framework. Consequently, new methods and new theory must be developed.

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.

Electron transport through nanometer-sized transistors based on carbon—a nanotube, a semiconductor nanowires or single molecules contacted by metallic electrodes take place according to the rules of quantum mechanics. Due to the strong Coulomb repulsion in these structures, this generally comprises a challenging, correlated, non-equilibrium many-body problem. In close collaboration with experimental groups both in-house and elsewhere, the condensed matter theory group maintains a strong effort to uncover new and explain already observed transport phenomena in these systems.

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, including the coherent quantum bits, 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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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 2016
The Solomon group’s activities were focused around our major project “Simulating Single-Molecule Pulling Experiments” under a Sapere Aude grant. Five PhD students and two postdocs are working on the project and we have had a number of exciting results. Our efforts resulted in 9 peer-reviewed publications for 2016.

GCS was honored to be appointed as a Löwdin lecturer by the Committee for Quantum Chemical Löwdin Lectures at Uppsala University. She gave her lecture at the MQM2016 Conference in Uppsala in June.

The Hansen group focuses on its major project “Charge Transfer and Catalysis in Metalloproteins” funded by the Lundbeck Foundation. With collaborators in Lund, Sweden TH finishes a project on the quantum dynamics of photosynthesis funded by the Swedish Research Council (VR).

In August, Gemma Solomon and Thorsten Hansen cohosted an International Workshop on: Charge, Heat and Energy Transport in Molecular Junctions celebrating the 60th birthday of Professor Vladimiro Mujica.
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 photovoltaics. 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 2016
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 which can 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.

With support from FTP, a project on photoswitchable liquid crystals is running. Another project on carbon-rich materials containing redox-active tetrathiafulvalenes is running with support from the Villum Foundation.

Molecular cruciform motifs were synthesized and subjected to single-molecule conductivity studies (conducting probe AFM and mechanically controlled break-junction (MCBJ) measurements in collaboration with Prof. Herre van der Zant at Delft University of Technology and the Nanochemistry group, Prof.s Bo W. Laursen and Kasper Nørgaard) – Published in J. Am. Chem. Soc. 2014, 136, 16457-16507.

KEYWORDS
Organic synthesis, Photoswitches, Redox-active Molecules, Solar energy

PEOPLE
Prof. Mogens Brøndsted Nielsen
3 Postdocs, 5 PhD students, approx. 10 students (BSc and MSc).

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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**

**PEOPLE**
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Nano Chemistry

In the Nano Chemistry Group, our research targets the design, synthesis and properties of novel graphene, metallic, organic and f-block containing materials for: molecular electronics, molecular self-assembly, fluorescent probes, and optical sensors. We published our work in both leading general journals: Nature Chemistry, JACS, Chemical Sciences, Chem. Comm., and more specialized journals: ACS Nano, Langmuir, and Advanced Materials. Our projects are highly interdisciplinary and involve collaboration with physicists, chemists, engineers, biologist as well as medical researchers locally in the NSC, in industry and at academic institutions across the globe. On the following two pages, you will find some examples of recent and on-going research in our group.

Fluorescent Dyes
Luminescent molecules play a vital role in medical and biological research due to their ability to sense, track and visualize DNA, proteins and other important biomolecules. The development of new, functional and more sensitive sensor molecules is a key activity in the Nano Chemistry Group. We have recently made two breakthroughs using our luminescent molecules. We were the first to demonstrate the use of near-infrared emission of lanthanide complexes to visualize objects in a confocal microscope (Chem Comm 2015). And we were the first to demonstrate intensity ratiometric sensing of oxygen, by using a molecular system with internal calibration (Chem Sci 2015). Detailed experimental and theoretical studies of the fundamental photophysical properties of pH sensitive rhodamine dyes have lead us to suggest a new model explaining the function of these important fluorescent indicators (Chem Eur J 2015).

Self-assembly of cationic pi-systems
When organic dyes are packed closely together, their optical properties are strongly depending on the exact structure. In some cases, such materials may act as antennas guiding light energy from large areas to specific molecules or guests in the system, similarly to what happens in the natural photosynthetic machinery. We design and synthesize new dyes with the ability to self-assemble into well-defined nanostructures (e.g. thin films, micelles or nanotubes) and study the relationship between the nanostructure and energy transport.
Ultra-thin and flexible electrodes for molecular electronics

The ultimate goal of molecular electronic research is to make nanoscale electronic components, where molecules play the role of transistors, memory bits and rectifiers. A major challenge in the field is how to create reliable electronic contact to the molecules. When metal contacts are used, short-circuits or damage to the fragile molecular active layer occur frequently. We have developed a method for fabricating and placing a few-nanometer thick layer of a flexible and highly conducting graphene film on top of a single layer of molecules. The thin graphene film protects the molecules and prevent short-circuits from forming.

Graphene technology

In collaboration with researchers from the Technical University of Denmark (DTU) and AU, the Nano Chemistry Group is partner in two large research projects with several industry partners on the use of graphene materials for industrial coatings and printed electronics. The projects have a total budget of DKK 65m (EUR 9m).

Carbonhagen

Since 2010, we have organized an annual international symposium on research and applications of carbon nanomaterials in collaboration with DTU Nanotech. The highly successful conference series with 150 participants in 2016, will continue in 2017 carbonhagen.com

The triazatriangulene (TATA) ring system was investigated as a binding group for tunnel junctions of molecular wires on gold surfaces. In this way, a new type of molecular device with the soft graphene electrodes have been developed (Advanced Materials 2012, 24, 1333–1339). We have further demonstrated how the optical transparency of the graphene film allows light to reach the active molecules in the nanodevice. By incorporating a light switchable molecule we were able to modulate the electrical conductance by light (Advanced Materials 2013, 25, 4164–4170.). Using the same nanoelectronic device structure, we have recently made bias switchable junctions of organic polymers (Nature Comm. 2015) We have been investigated a new anchoring group for molecular electronics, based on a triazatriangulene (TATA) platform system. We demonstrated that despite the presence of a sp³ hybridized carbon atom in the conduction path, the TATA platform displays a contact resistance only slightly larger than commonly used thiols (Langmuir 2014).

KEYWORDS

Molecular electronics, organic synthesis, graphene materials, fluorescent dyes and sensors, lanthanide chemistry, self-assembling nanostructures, and surface

PEOPLE

Professor Bo W. Laursen, Associate Professors Kasper Nørgaard and Thomas Just Sørensen, 4 postdocs, 6 PhD students, 10 undergraduates.

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The primary focus of our lab is to provide the molecular level mechanisms that underlie and control protein behavior with emphasis on structure function correlations and biomolecular interactions. The ultimate target is to utilize the attained knowledge for improving human health and for the design of tailor made biocatalysts for biotechnological, green energy, solutions. To succeed in this, and often inspired by nature, we develop biophysical assays in native-like membrane environments and employ biophysical tools that allow molecular interrogations with the unprecedented sensitivity of single-molecule readouts.

Focusing on a spectrum of biological systems, we investigate how the personality of a nanometer-dimension enzyme propagates to biological phenomena. As such, interrogating the structural and functional dynamics of an enzyme allows us to provide links between nanometer motions and ultrafast structural dynamics to human diseases, clinical phenotypes and industrial performance (e.g. detergents in industry). In a way, we strive to provide links of protein landscapes to clinical and industrial phenotypes. All our projects are in tight collaboration with industrial partners (e.g. Novozymes), medical doctors, and biological labs and are at the interface between biology, medicine and clinical biochemistry.

In 2015, Nikos S Hatzakis was awarded the prestigious Villum Young Investigator funding, that is directed to especially talented up-and-coming researchers in science and technology with ambitions of creating their own, independent research identity. With this grant, we equipped our lab with state-of-the-art super-resolution tools.
In 2017 Nikos S Hatzakis was awarded the prestigious “Distinguished Associate professor fellowship” from Carlsberg foundation, that supports outstanding newly appointed associate professors with international experience to establish an independent research group or environment. The fellowship is on “Role of conformational DYNamics on enzyme FUNCTION (from single molecule insights to Rational de novo protein design)” With this grant we will equip our microscopes with state of the art add-ons, hire new personal and establish new collaboration with protein re-design experts.

SELECTED PUBLICATIONS

PEOPLE
Nikos Hatzakis, Min Zhang, Pradeep Kumar Singh, Yi Long, Matias Moses, Soren Nielsen, Camilla Thorlaksen, Simon Bo Jensen, Mette G Malle, Julie Dihtmar.

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We are a young group at the Nano-Science 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.

However, the effect of nanosizing on the atomic arrangement of the materials is very poorly understood. 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 new synthesis methods, high-energy synchrotron X-ray radiation as well as newly developed scattering techniques for nanostructure analysis, we work on elucidating the structure of complex nanomaterials, e.g. noble metal nanoclusters as illustrated in Figure 1. Our main method is Total Scattering and Pair Distribution Function (PDF) analysis, which goes beyond traditional crystallographic methods for structure analysis and allows us to determine the atomic arrangements in nanomaterials. Apart from studying the structure of nanoparticles, we are also able to follow material synthesis in situ to get a glimpse of nanostructure formation and elucidating fundamental reaction mechanisms in nanochemistry. Figure 2 shows time resolved scattering data from the growth of metal oxide clusters in solution.

We study a broad range of energy materials, with

Nanomaterials by design

With the recent developments in nanochemistry, chemists and material scientists are becoming better and better at engineering materials on the nanoscale, and nanoparticles of e.g. metal and metal oxides can now be synthesized with very high precision, opening for a range of applications in energy storage and conversion.
applications in solar cells, batteries, catalysis. We are frequent users of synchrotron and neutron facilities in Europe and the US, and a significant part of our experimental work takes place at these large-scale facilities. By means of collaborations in both Europe and the US, we are part of the development of new methods for nanostructure characterization.

In situ X-ray scattering allows us to follow the formation of nanoclusters in solution.

**KEYWORDS**

**SELECTED PUBLICATIONS**

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

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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, CO$_2$, O$_2$, 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 CO$_2$ 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, AECOM and Arcadis.

We have expertise and instrument facilities that are unique in the world for characterising natural materials at nanometre scale, for example, X-ray photoelectron spectroscopy (XPS), focused ion beam scanning electron microscopy (FIB-SEM) and atomic force microscopy (AFM) with chemical force mapping (CFM). We are frequent users of a range of techniques at synchrotron radiation (SR) facilities around the world, such as X-ray tomography (XCT) and we make good use of computational approaches, including molecular dynamics (MD) and density functional theory (DFT). Our newest instrument, an AFM-IR, is based on atomic force microscopy (AFM), which maps topography on surfaces with nanometre resolution laterally and subnanometre resolution perpendicular to the surface. Coupled to the AFM is a pulsed, tuneable infrared (IR) laser. Material on the sur-
Surface can be detected by the tip when the wavelength of the laser matches its absorption energy. We can record IR spectra at chosen surface sites, for fingerprinting, or we can select a wavelength and map material that absorbs energy at that specific wavelength, for example, O-H, N-H and C-H stretching in the 2,700 to 3,600 cm⁻¹ range. We are using AFM-IR to characterise the organic material that adsorbs on all solid surfaces.

X-ray micro and nanotomography (XCT) provides 3D images of the micro and nanometre scale structure of materials without destroying the sample. This is useful for time dependent studies, when the material is fragile or when analysis with several techniques is required. One of our large projects, Predicting Petrophysical Parameters (P3), funded by Maersk Oil and the Danish Innovation Foundation, aims to derive information from drill cuttings, about pore networks and the flow of oil and water, to optimise production strategies. Microstructural characterisation of soil and aquifer material can contribute to groundwater protection or remediation of contaminated sites. Using the 3D tomography images, we can model the behaviour of CO₂ as it displaces water in the pore networks of rocks, for example, to test the long term effects of CO₂ injection, underground in chalk, such as in the North Sea oil fields (CINEMA Project) and in basalt (Carb-Fix Project).

in Iceland, where CO₂ has been shown[6] to react to form secondary minerals, thus trapping it for geological time scales. 3D images from a sample of chalk from the North Sea Basin (103 µm³) where modelling predicts how the flow of CO₂ (red) would displace water (grey) (Gooya et al., work in progress).

Metal-Aid, a new European Commission ITN (International Training Network) began in late 2016. It will train 14 PhD students in 5 countries in an integrated effort that will join researchers at 6 universities, 4 consulting engineering firms and a government agency. The goal is to develop natural nanoparticles called "green rust" (photo, top of this page) that will trap contaminants[2], such as heavy metals, and degrade organic compounds from soil and groundwater, in situ.

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 Research, Technical and Admin. Associates and Assistants; 12 Postdoctoral Fellows; 15 PhD, several Master and Bachelor Students; 2 Guest Researchers.

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Nanopharmaceutics

Vito Foderà and Marco van de Weert are from the Protein Formulation and Biophysics group at the Department of Pharmacy, UCPH. The group’s focus is on unraveling the mechanisms of destabilization of proteins due to interactions with their surroundings, with focus on protein self-assembly into nanostructures and microstructures. We aim at developing experimental and theoretical platforms to control the 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 methods with advanced analysis of X-ray scattering data and imaging. Theoretical models are also developed for the quantitative analysis of the experimental data.

Hanne Mørck Nielsen, Peptide and Protein Drug Delivery group at Department of Pharmacy, UCPH. We strive to elucidate the interplay between macromolecular therapeutics and biological barriers in order to advance therapy with peptide and protein drugs. Specifically, projects relate to studying molecular interactions between molecules in drug delivery systems designed for specific routes of administration, property characterization of self-assembled drug delivery systems, nanoparticles and microparticles, gels etc. We take a mechanistic approach to understanding the detailed interplay between the drugs, excipients, drug delivery systems, and biobarriers seen in a global perspective. The studies are done with a refined toolbox of models for drug absorption, metabolism and compatibility exploiting the use of e.g. molecular engineered excipients like cell-penetrating peptides and hyaluronic acid for improving drug delivery.

**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 microsized drug delivery systems, Membrane interaction, uptake and transport, Mucus interactions, Cell culture models

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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 10 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, engineered nanoparticles and nanomedicine. The most important mechanisms of action are oxidative stress, inflammation, genotoxicity and vascular dysfunction.

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 improve public health 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 biological measurements 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, Organicsynthesis, Catalysis, Chirality

**SELECTED PUBLICATIONS**

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

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How to create, control, measure and protect quantum coherence and entanglement in solid state electronic devices is the main theme of the Center for Quantum Devices, funded by the Danish National Research Foundation. Specific systems investigated include devices in III-V and group-IV semiconductors, coupled electron-nuclear systems, carbon based electronics and Majorana fermion systems realized in nanowires and two-dimensional electron gases coupled to superconductors. Moreover, within the Nano-Science Center we develop novel biosensors in collaboration with the Bionanotechnology group, Raman imaging with Nano Spectroscopy as well as graphene and molecular electronics with Nano Chemistry.

Facilities Central to the Center is its coordinated activity in materials growth, nanoscale fabrication, GHz-bandwidth measurements at millikelvin temperatures, numerical simulation and theoretical prediction and interpretation. The group hosts a cleanroom with a suite of nanofabrication tools, including molecular beam epitaxy, scanning and transmission electron microscopes and two electron beam lithography systems.

**KEYWORDS**
Quantum entanglement, quantum coherence, topological systems, quantum dots, quantum Hall systems, Majorana fermions, nanowires, nanotubes, nanoelectronics, superconductors, condensed matter physics, sensors

**PEOPLE**
8 Professors and Associate Professors, 14 postdocs, 18 PhD students, 25 MSc and BSc students.

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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 2016:
- 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 Sustainable 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

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 Roquelle

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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.

Highlights from 2016:
A number of studies rely on the controlled contrast for neutron scattering. Contrast variation is however also possible in X-ray scattering [1,2]. Many studies concern the interaction between magnetism and superconductivity. Another study has revealed an unusual “rotor” mode in nanoparticles, which may be seen as a high-temperature analog to superparamagnetism.

The dynamics of hydrogen is crucial for wide ranges of systems, ranging from the biological function of life to new building materials. Inelastic neutron scattering methods is ideal for such studies, and we have demonstrate that the development of nanoscale hydrogen bonded network is the key to the performance of new “green-materials” [3]. Protein and peptide based nanodiscs have emerged as
a platform for studying membrane proteins [1]. We have developed a peptide system that mimic A1 based lipoprotein with respect to its solution properties. The structure, as determined by combined SAXS and SANS, reveals a discoidal shape, thus providing a new platform for large membrane protein complexes. Other studies concern the dynamics of protons in organic as well as inorganic materials [3]. Conventional X-ray transmission radiography relying on the absorption contrast is well known and established. Much better resolution can be obtained using x-ray tomography based on the full complex index of refraction, i.e. recording absorption and phase-contrasts or scattering. Such concepts were demonstrated by experimental results in nanomaterials as well as in food products [4].

NBI is involved in a number of design studies and proposal of instruments for ESS. Several of these studies have been approved by ESS to be among the first instruments to be constructed [5].

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

**SELECTED PUBLICATIONS**

**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 Udby and Jacob Kirkengaard. 6 postdocs and 25 PhD students.

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