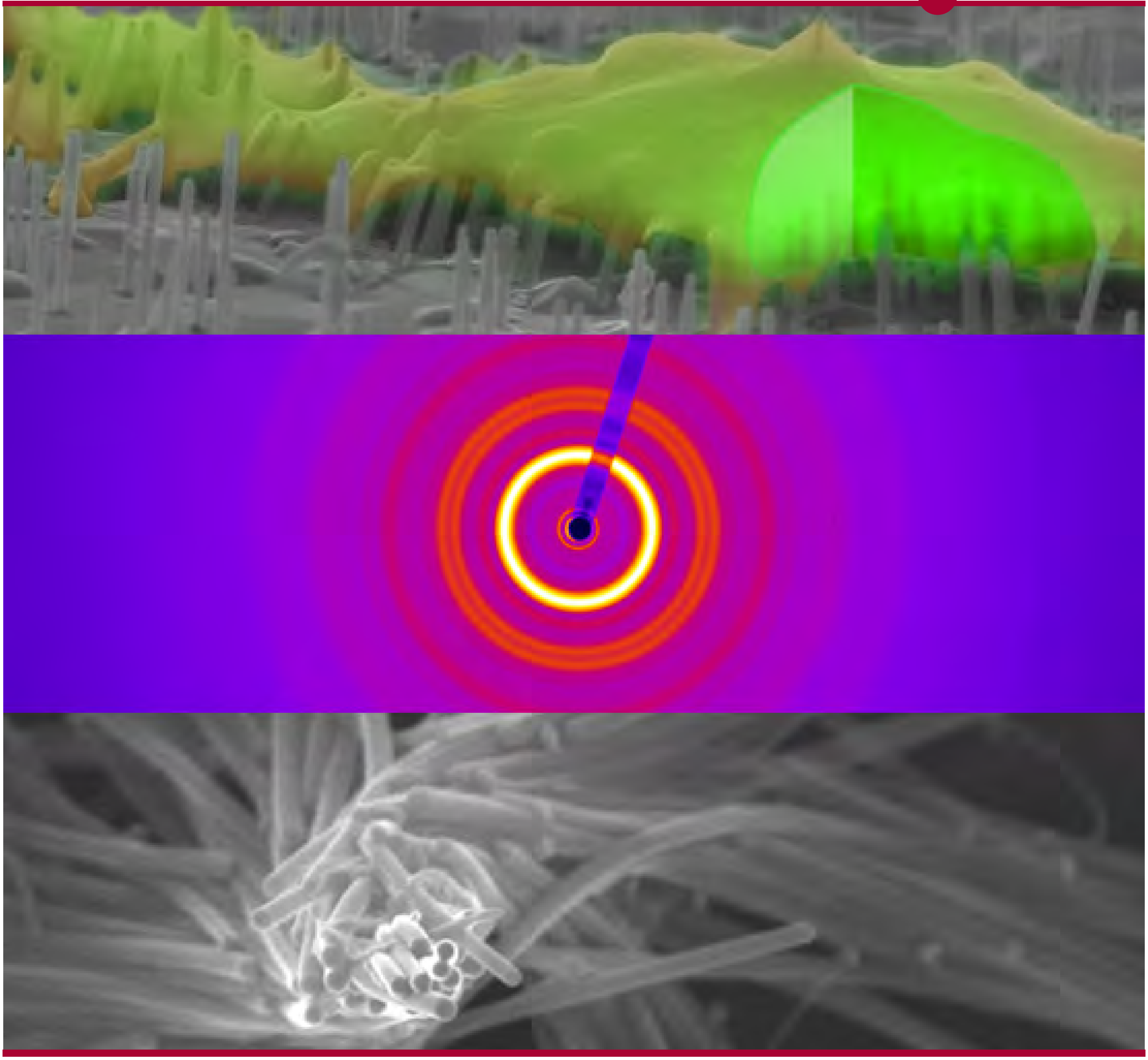
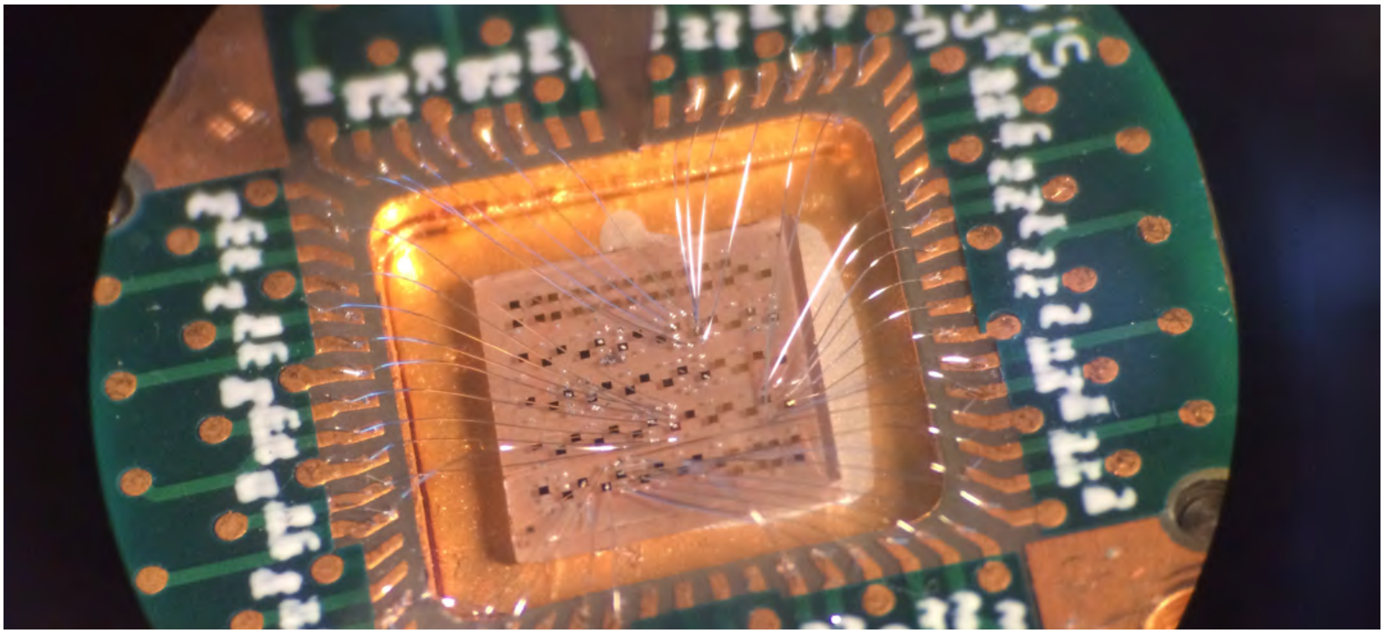
NANO-SCIENCE CENTER

UNIVERSITY OF COPENHAGEN



Annual Report 2015



Frontcover

Top: Mammalian cells cultured on a forest of semiconductor nanowires. Collaboration between the Bio-Nanotechnology lab and Center for Quantum Devices, Nano-Science Center. Micrograph and illustration by Trine Berthing. The image has appeared at the cover of the journal ***Small***.
Middle: X-ray scattering pattern from 2 nm gold nanoclusters.
Bottom: Bundle of InAs nanowires. Scanning electron micrograph by Rawa Tanta, Center for Quantum Devices.

Backcover

Cryogenic probe station used to test quantum devices in vacuum at low temperatures. An electronic chip is visible in the center of the platform. From Center for Quantum Devices.

Colophon

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instagram.com/scienceku

youtube.com/user/sciencecopenhagen

twitter.com/science_ku

Contents

2015 in short

Highlights of the Nano-Science Center activities include:

• The nanoscience undergraduate programme reached its all-time high in 2015 with 68 students enrolled in September, and 11 new international students joined the master's programme.

• 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 NSC and the iNANO at Aarhus University.

• Eleven 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.

• In August, the Nano-Science Center co-hosted the 6th international symposium Carbonhagen together with DTU Nanotech and reached 160 participants in 2015.

• Educationbased research: In July, Associate professor Thomas Just Sørensen and all first-year nanoscience students from the course Nano1 published a peer-reviewed research paper in ***Chem. Nano. Mat.*** on self-assembly. The article shows great potential in the intimate mixing of research and education leading to both valuable research results and highly motivating education.

• Attracting new researchers
Three new research groups have been formed by attracting research talents.

Associate Professor Nikos Hatzakis formed the group Nanoenzymology.

New tenure-track Assistant Professor Kirsten Ørnsbjerg Jensen was reqruited from Columbia University in New York to form the new group in Nanomaterial Structure.

Jan Rossmeisl, former DTU was appointed new Professor in chemistry at University of Copenhagen and joined the NSC with his group Theoretical Catalysis.

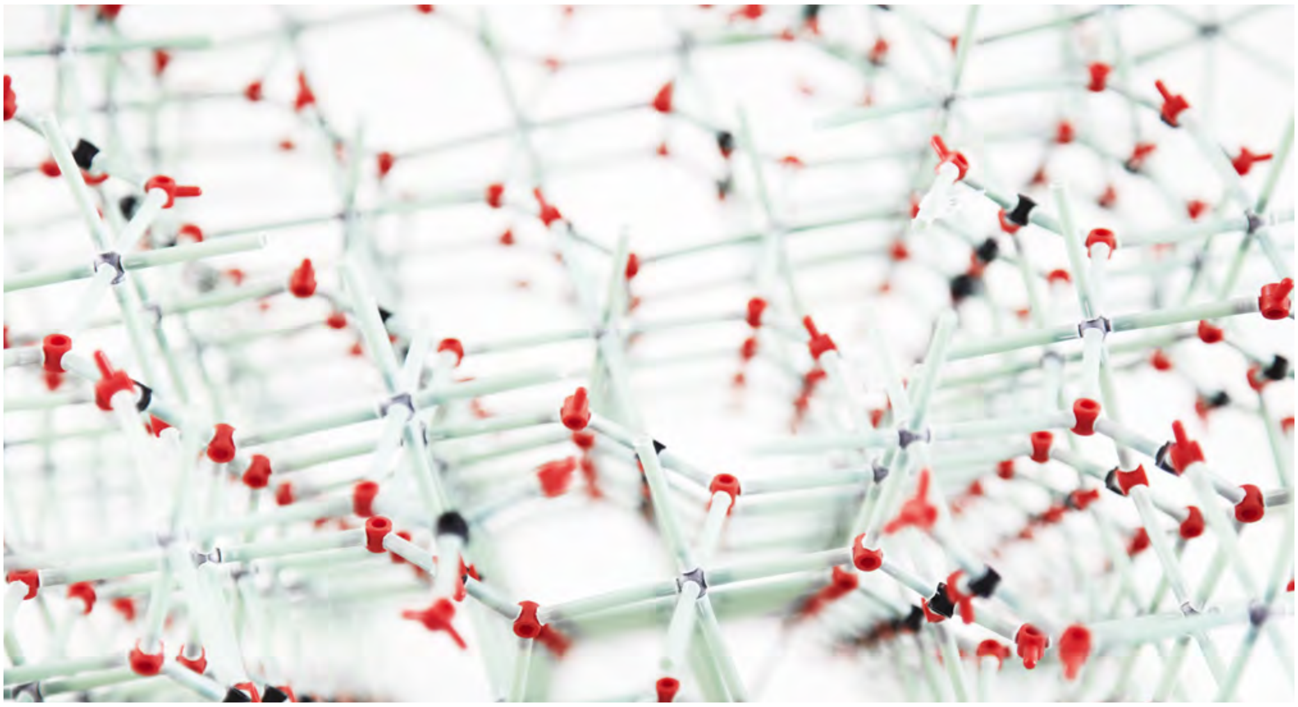
Happy reading

Bo Wegge Laursen and Tine Buskjær Nielsen

What is nanoscience?

Nanos means 'dwarf' in Greek. Nano is used as a prefix and means 'one billionth of', or 10^{-9}. So 1nm is 0.000000001 metre. A human hair is approximately 80,000 nanometres in diameter.

Nanoscience studies atoms, molecules and objects in the nm size range, 1-100 nm. The invention of the scanning tunneling microscope in 1981 made way for studying objects at the nanoscale. The microscope is not "seeing" small stuff but "feeling" its way forward with a tiny needle. Since then, chemists, physicists, biologists and others have joined in with using the same methods and instruments, so nanoscience has been an interdisciplinary research field from the very beginning.



What is the Nano-Science Center?

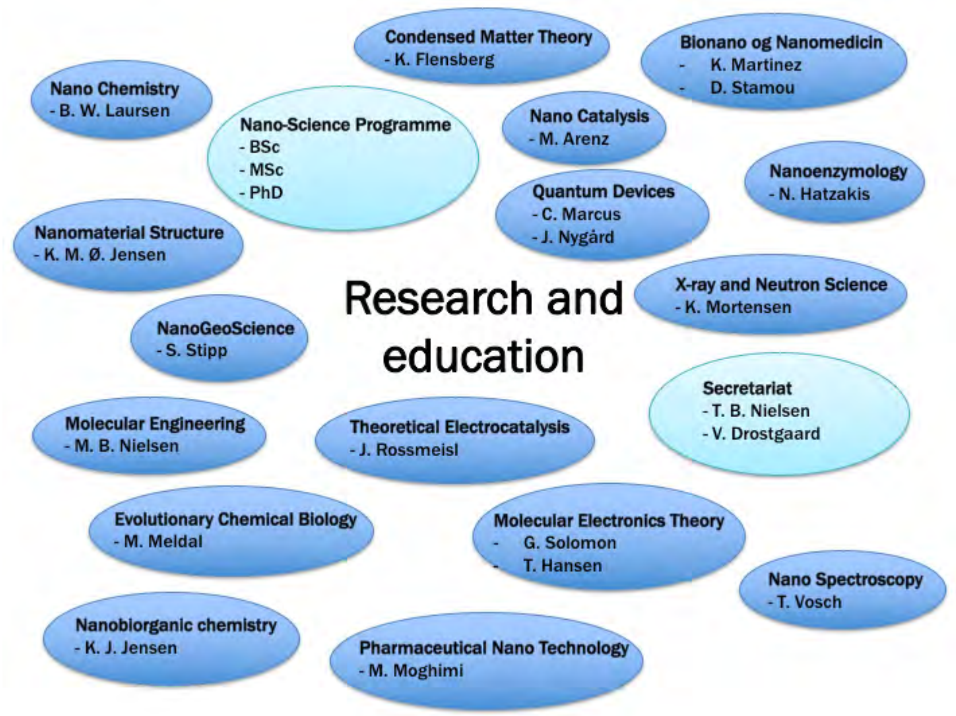
The Nano-Science Center with the University of Copenhagen is one the world's leading research environments for nanoscience. More than 200 researchers from classical research areas like physics, chemistry, biology and medical sciences are members of the center linking the Faculty of Science and the Faculty of Health and Medical Sciences. The broad range of research groups in the 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.

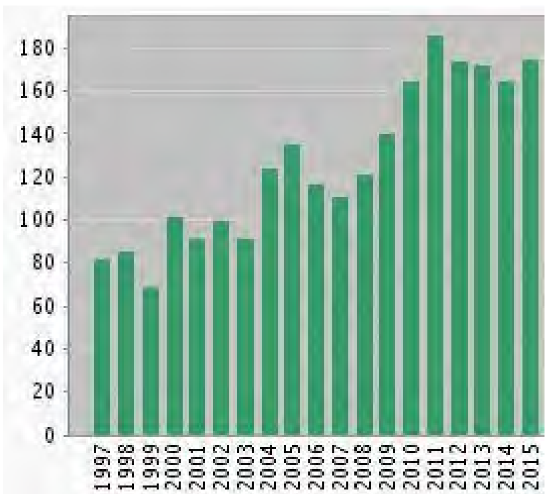
Nano-Science Center



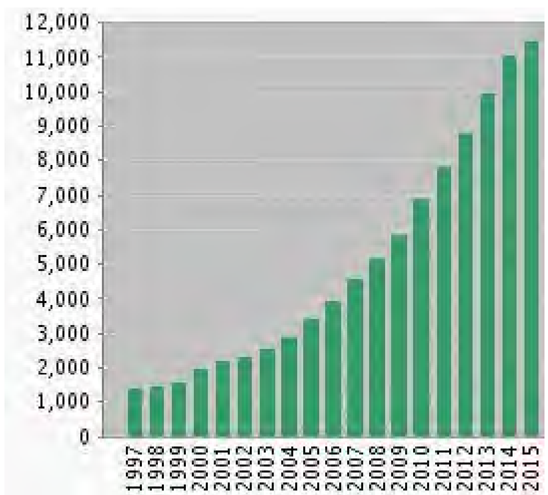
Publications and Citations

In 2015, researchers from the Nano-Science Center succesfully published more than 170 peer-reviewed papers. Their works were cited more than 11,000 times in research media.

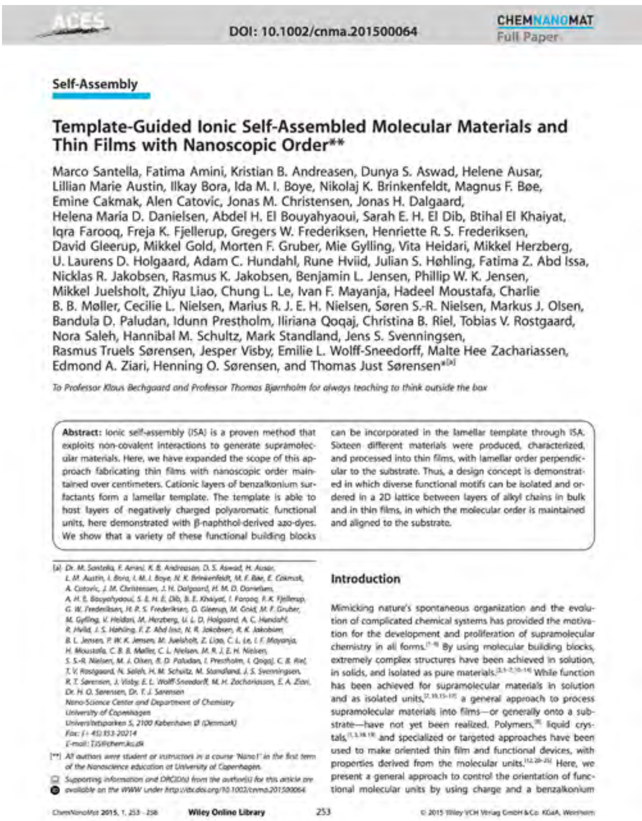
Published Items in Each Year



Citations in Each Year



First-year students become researchers from day one



DOI: 10.1002/cnma.201500064 CHEMNANOMAT Full Paper

Self-Assembly

Template-Guided Ionic Self-Assembled Molecular Materials and Thin Films with Nanoscopic Order**

Marco Santella, Fatima Amini, Kristian B. Andreasen, Dunya S. Aswad, Helene Ausar, Lillian Marie Austin, Ilkay Bora, Ida M. I. Boye, Nikolaj K. Brinkenfeldt, Magnus F. Bøe, Emine Cakmak, Alen Catovic, Jonas M. Christensen, Jonas H. Dalgaard, Helena Maria D. Danielsen, Abdel H. El Bouyahyaoui, Sarah E. H. El Dib, Btihal El Khaiyat, Iqra Farooq, Freja K. Fjellerup, Gregers W. Frederiksen, Henriette R. S. Frederiksen, David Gleerup, Mikkel Gold, Morten F. Gruber, Mie Gylling, Vita Heidari, Mikkel Herzberg, U. Laurens D. Holgaard, Adam C. Hundahl, Rune Hviid, Julian S. Høhling, Fatima Z. Abd Issa, Nicklas R. Jakobsen, Rasmus K. Jakobsen, Benjamin L. Jensen, Phillip W. K. Jensen, Mikkel Juelsholt, Zhiyu Liao, Chung L. Le, Ivan F. Mayanja, Hadeel Moustafa, Charlie B. B. Møller, Cecilie L. Nielsen, Marius R. J. E. H. Nielsen, Søren S.-R. Nielsen, Markus J. Olsen, Bandula D. Paludan, Idunn Prestholm, Iliriana Qoqaj, Christina B. Riel, Tobias V. Rostgaard, Nora Saleh, Hannibal M. Schultz, Mark Standland, Jens S. Svenningsen, Rasmus Truels Sørensen, Jesper Visby, Emilie L. Wolff-Sneedorff, Malte Hee Zachariassen, Edmond A. Ziari, Henning O. Sørensen, and Thomas Just Sørensen*[a]

To Professor Klaus Bechgaard and Professor Thomas Bjørnholm for always teaching to think outside the box

Abstract: Ionic self-assembly (ISA) is a proven method that exploits non-covalent interactions to generate supramolecular materials. Here, we have expanded the scope of this approach fabricating thin films with nanoscopic order maintained over centimeters. Cationic layers of benzalkonium surfactants form a lamellar template. The template is able to host layers of negatively charged polyaromatic functional units, here demonstrated with β-naphthol-derived azo-dyes. We show that a variety of these functional building blocks can be incorporated in the lamellar template through ISA. Sixteen different materials were produced, characterized, and processed into thin films, with lamellar order perpendicular to the substrate. Thus, a design concept is demonstrated in which diverse functional motifs can be isolated and ordered in a 2D lattice between layers of alkyl chains in bulk and in thin films, in which the molecular order is maintained and aligned to the substrate.

Introduction

Mimicking nature's spontaneous organization and the evolution of complicated chemical systems has provided the motivation for the development and proliferation of supramolecular chemistry in all forms.[1–9] By using molecular building blocks, extremely complex structures have been achieved in solution, in solids, and isolated as pure materials.[2,5–7,10–14] While function has been achieved for supramolecular materials in solution and as isolated units,[7,10,15–17] a general approach to process supramolecular materials into films—or generally onto a substrate—have not yet been realized. Polymers,[8] liquid crystals,[1,3,18,19] and specialized or targeted approaches have been used to make oriented thin film and functional devices, with properties derived from the molecular units.[12,20–25] Here, we present a general approach to control the orientation of functional molecular units by using charge and a benzalkonium

[a] Dr. M. Santella, F. Amini, K. B. Andreasen, D. S. Aswad, H. Ausar, L. M. Austin, I. Bora, I. M. I. Boye, N. K. Brinkenfeldt, M. F. Bøe, E. Cakmak, A. Catovic, J. M. Christensen, J. H. Dalgaard, H. M. D. Danielsen, A. H. E. Bouyahyaoui, S. E. H. E. Dib, B. E. Khaiyat, I. Farooq, F. K. Fjellerup, G. W. Frederiksen, H. R. S. Frederiksen, D. Gleerup, M. Gold, M. F. Gruber, M. Gylling, V. Heidari, M. Herzberg, U. L. D. Holgaard, A. C. Hundahl, R. Hviid, J. S. Høhling, F. Z. Abd Issa, N. R. Jakobsen, R. K. Jakobsen, B. L. Jensen, P. W. K. Jensen, M. Juelsholt, Z. Liao, C. L. Le, I. F. Mayanja, H. Moustafa, C. B. B. Møller, C. L. Nielsen, M. R. J. E. H. Nielsen, S. S.-R. Nielsen, M. J. Olsen, B. D. Paludan, I. Prestholm, I. Qoqaj, C. B. Riel, T. V. Rostgaard, N. Saleh, H. M. Schultz, M. Standland, J. S. Svenningsen, R. T. Sørensen, J. Visby, E. L. Wolff-Sneedorff, M. H. Zachariassen, E. A. Ziari, Dr. H. O. Sørensen, Dr. T. J. Sørensen
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[**] All authors were student or instructors in a course "Nano1" in the first term of the Nanoscience education at University of Copenhagen.

Supporting information and ORCID(s) from the author(s) for this article are available on the WWW under http://dx.doi.org/10.1002/cnma.201500064.

ChemNanoMat 2015, 1, 253 – 258 Wiley Online Library 253

08/NATIONALT

Lektor Thomas Just Sørensen og studerende Ida Marie Ingmer Boye har sammen med de øvrige nanostuderende på årgang 2013 på Københavns Universitet forsket sig frem til et gennembrud i nanoteknologien, som er så epokegørende, at et videnskabeligt tidsskrift nu bringer en artikel om deres forskningsresultat. Foto: Claus Bech

Studerende springer ud som forskere

Blåstemplet. I denne uge udgives et nyt forskningsresultat, som førsteårsstuderende på nanoscience på Københavns Universitet står bag. De lærte at forske, før de havde lært den grundlæggende teori.

Af Bodil Jensen

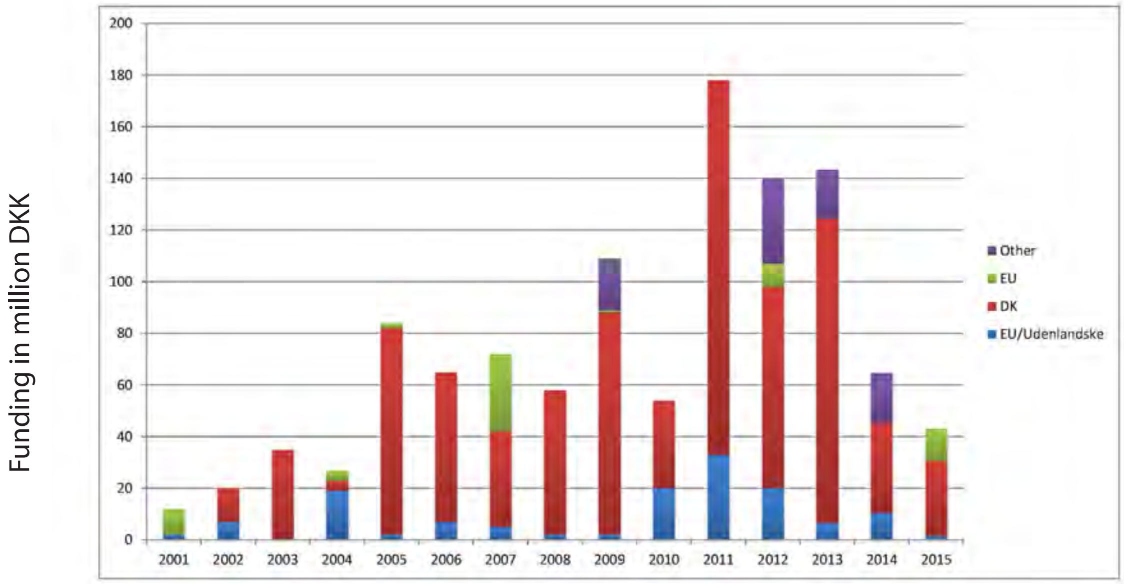
"Template-Guided Ionic Self-Assembled Molecular Materials and Thin Films with Nanoscopic Order"
Marco Santella et al., ***Chem. Nano. Mat.***, 2015, 1, 254-258.
DOI: 10.1002/cnma.201500064.

Article in Berlingske regarding reaserch project by Associate Professor Thomas Just Sørensen and first-year students in the course Nano1.

Associate Professor Thomas Just Sørensen transformed the first-year course Nano1 into a research programme where students designed, executed and analyzed experiments.
In 2015 that resulted in an entire class co-authoring a scientific paper on self-assembling molecular electronics using nanoscience. The students have developed a simple process to control what is known as self-assembling molecular electronics. Their breakthrough can make a difference in the development of low-cost, powerful solar energy facilities, as well as in screen technology, and in the development of more environmentally sustainable electronic devices. The successful combination of teaching and open-ended research also gained signifcant attention in the public as an example of teaching-based research.

External funding

During 2015, the research groups in NSC 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 2015:

Maersk Olie og Gas	Niras	Gubra aps
BP	COWL	Novartis
DONG Energy	GEO	Quantumwise
Reykjavik Energy	Applied Biomimetic	Hempel
Rockwool	BMW	Medtronic
Haldor Topsøe	Novo Nordisk	Novozymes

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.

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.

Eleven 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.

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

Graduated PhD’s in 2015

Klaus Martin Sigild Juhl
“Adhesion Properties of Organic Compounds to Oxide Surfaces“

Tania Kjellerup Lind
“Understanding Peptide Dendrimer Interactions with Model Cell Membrane Mimics“

Qian Li
“Electron and phonon transport in molecular junctions“

Nini Elisabeth Abildgaard Reeler
“Self-Assembly on Gold and Graphene for Molecular Electronics“

Morten Kjærgaard
“Proximity Induced Superconducting Properties in One and Two Dimensional Semiconductors“

Ilkay Bora
“Development And Characterization Of Reactive Triangulenium Chromophores For Bioconjugation Applications”

Marco Santella
“Synthesis, Optical Properties and Applications for New Triangleniums Derivatives“

Salome Veshaguri
“Proton pumping and slippage dynamics of a eukaryotic P-type ATPase studied at the singlemolecule level“

Pie Huda
“Studying membrane protein structure and function using nanodiscs“

Murillo Longo Martins
“Synthesis and characterization of a bionanocomposite for cancer treatment“

Andrew Higginbotham
“Quantum Dots for Conventional and Topological Qubits“

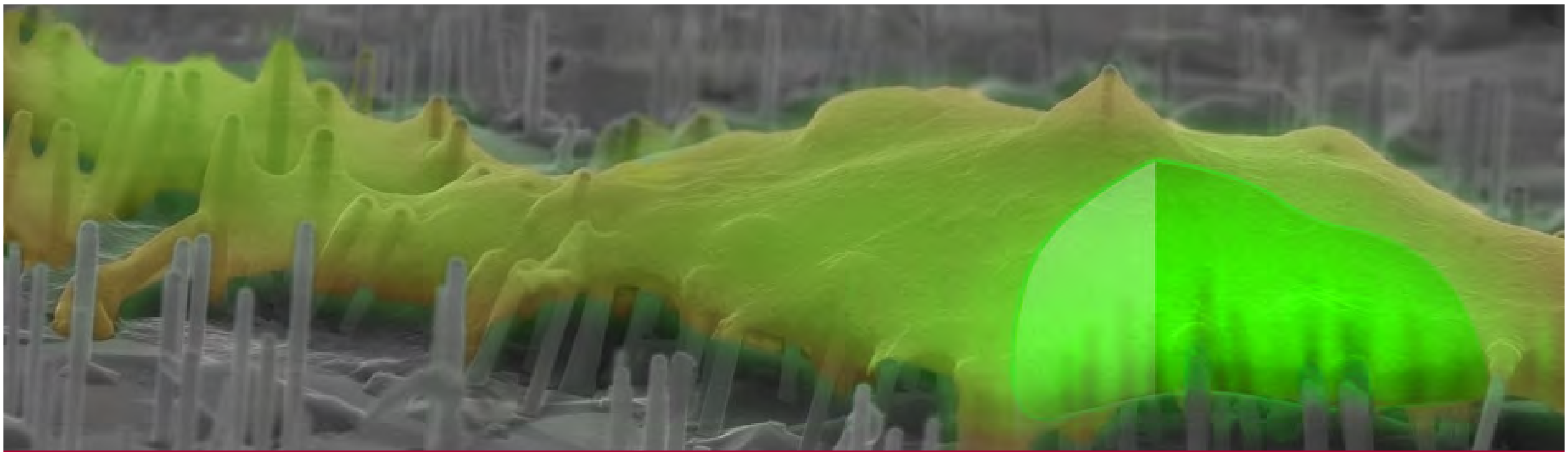
Anders Sebastian Rosenkrans Ødum
“Processing Proteases“

Jerome Mlack
“Growth and Low Temperature Transport Measurements of Pure and Doped Bismuth Selenide “

Astrid Tranum Rømer
“Spin- uctuation mediated superconductivity and magnetic order in the cuprate La1:88Sr0:12CuO4“

Maria Thomsen
“Subcutaneous injections:
Visualising and optimising device-tissue interactions“

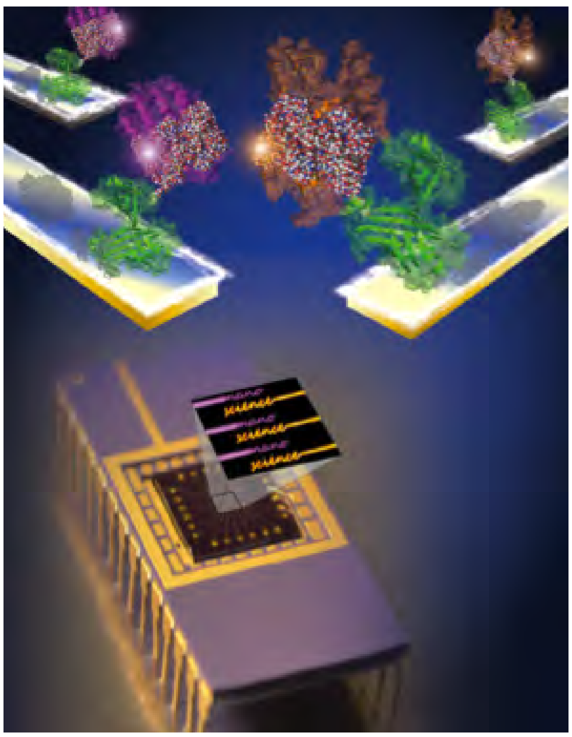
Konrad Udo Hannes Wölms
“Aspects of Majorana Bound States in One-Dimensional Systems with and without Time-Reversal Symmetry“



Bionanotechnology and Nanomedicine - Martinez group

The group exploits novel nanotechnologies and biophysical 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.



Nanoelectrodes selectively functionalized with distinct membrane proteins (Della Pia et al. ACS nano 2014)

Highlights from 2015

- We have published the 1st review in the field of "interface of high-aspect-ratio nanostructures with living cells" (Bonde et al. 2014 ***Nanotechnology***).
- Novel optical properties of vertical arrays of InAs nanowires have been revealed in collaboration with the groups of J. Nygård, T. Vosch and A. Foncuberta I Moral (EPFL).
- A new platform with nanoelectrodes suitable for membrane proteins multiplexed nanoarrays (DellaPia et al. 2014 ***ACS Nano***) has been developed in collaboration with J. Nygård's group.
- New properties of amphipatic polymers (amphipols) for membrane protein immobilization on surfaces have been illustrated in collaboration with M. Zoonens (Paris).
- This year, 1 PhD student, 3 Master students and 2 Bachelor students graduated in our group.

Keywords

Bionanosensors, nanowires, nanoparticles, nanoelectrodes, membrane proteins, GPCRs, amphipols and nanodiscs, surface sensitive techniques, cellular studies.

Selected Publications

[1] E.A Della Pia et al. ***ACS nano*** 2014, 8 (2), 1844-1853

[2] R. Frederiksen et al. ***Nanoletters*** 2015 15 (1), 176–181

[3] S. Bonde et al. , ***Nanotechnology*** 2014; 25, 362001

[4] E. A. Della Pia et al. ***J. Membr. Biol.*** 2014; 247, 815-826

People

Associate Prof. K. L. Martinez, 4 postdocs and 5 PhD students

Contact

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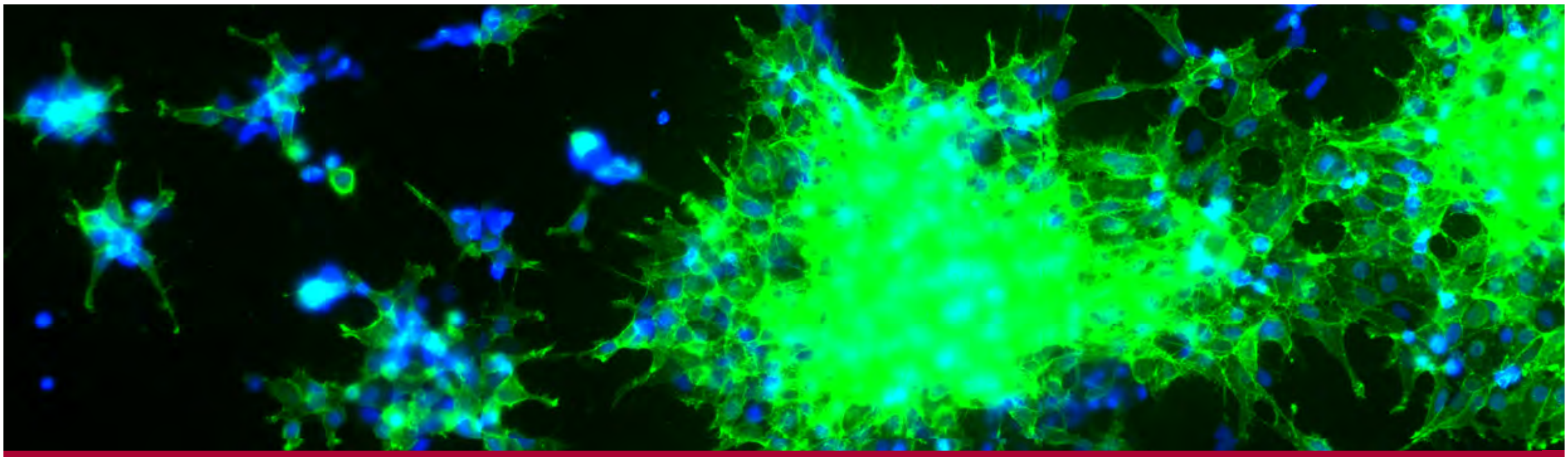
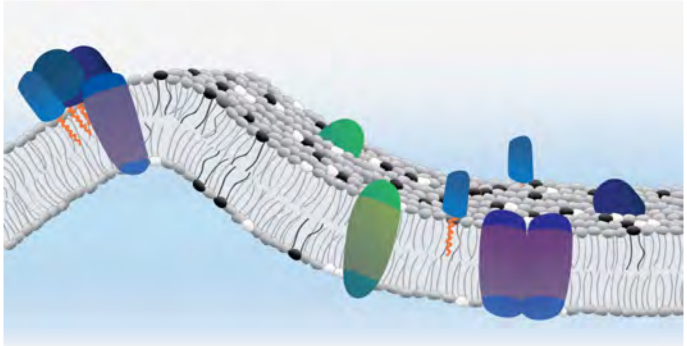


Bionanotechnology and Nanomedicine - Stamou Group

Our main research interest is the spatio-temporal organization of biological systems on the nanoscale and its impact on normal and aberrant biological functions.
A plethora of protein-protein interactions take place at membrane interfaces and within the heterogeneous lipid matrix itself. Using reconstituted and native lipid membranes, the group tries to understand the nature of the influence of nanoscale membrane composition, internal structure, shape, etc. on the interactions of trans- membrane proteins (e.g. oligomerization) and membrane-associated proteins. Systems studied include GPCRs, scaffoalding proteins, the SNARE complex, BAR domains and protein coats.



A plethora of biological processes take place on or near cellular membranes. At the Bionano lab we investigate many such processes on the nanoscale using novel tools and methods.

The problems we are trying to solve are situated at the interface of biology, physics and nanotechnology, and to address them experimentally we have assembled a highly interdiscplinary group that includes molecular biologists, biochemists, physicists, nanotechnologists and material scientists. Our core expertise is advanced biofunctional surfaces that we use to isolate in a controlled environment from single molecules up to reconstituted signaling complexes, and quantitative optical microscopies that we use in combination with a number of other surface-sensitive techniques to characterize our samples.

Many of our projects are carried out in close collaboration with groups that specialize in protein purification and reconstitution, structural characterization, molecular dynamics simulations or theory.

A part of our group is harnessing our expertise on self-assembly and quantitative microscopy in order to develop prototypic biosensing nanoscale platforms and zeptolitre fluidic devices for applications in screening and diagnostics.

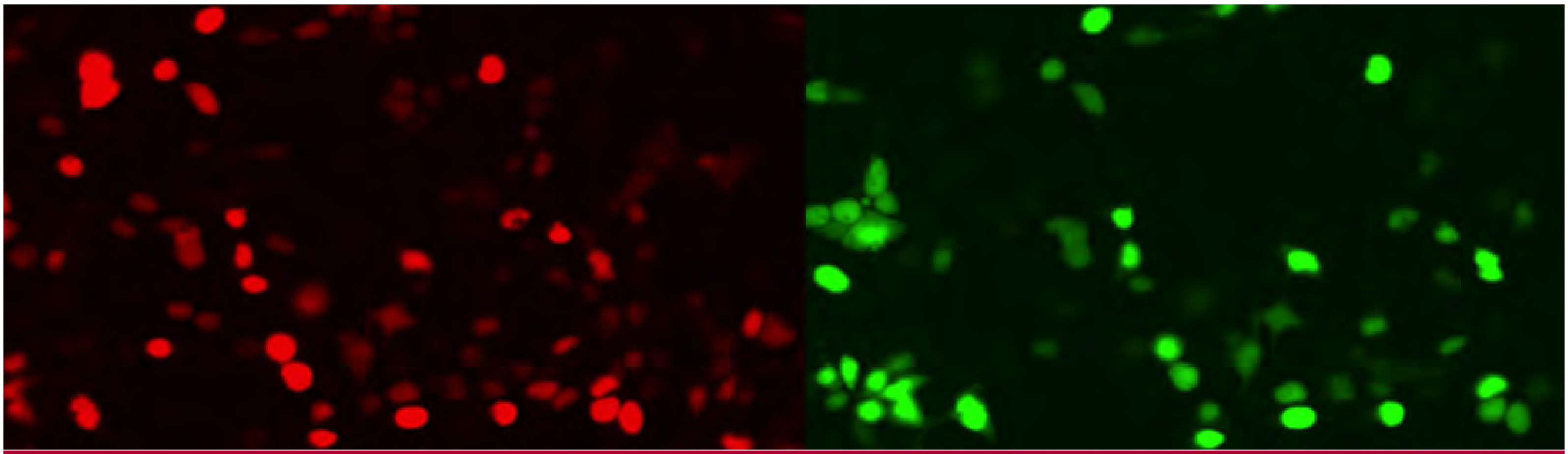
Keywords
Protein-membrane interactions, nanoscale membrane biophysics, fluorescence microscopy, single molecule techniques, biologically inspired nanoscale sensors and fluidics

Selected Publications

[1] Jannik Bruun Larsen et al., ***Nat. Chem. Biol.***, 2015. 11 (3): p. 192-194, Front Cover Page
[2] Signe Mathiasen et al., ***Nat. Methods***, 2014. 11 (9): p. 931-934
[3] L. Iversen, et al., ***Science***, 2014, 345 (6192): p. 50-54
[4] S. M. Christensen, et al., ***Nat. Nanotechnol.***, 2011. 7 (1): p. 51–55
[5] N. S. Hatzakis, et al., ***Nat. Chem. Biol.***, 2009. 5 (11): p. 835, – Highlighted in a News and Views Article in Nature Chemical Biology. 2009. 5 (11): p. 783
[6] P. M. Bendix, et al., ***Proc. Natl. Acad. of Sci.***, 2009. 106 (30): p. 12341

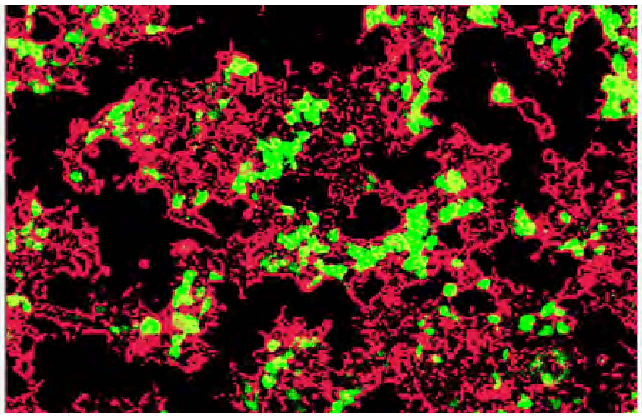
People
Prof. D. Stamou, ~5 postdocs and ~5 PhD students, 1 administrator.

Contact
Dimitrios Stamou, stamou@nano.ku.dk



Center for Evolutionary Chemical Biology

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 platform for expression YFP upon GPCR activation

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.

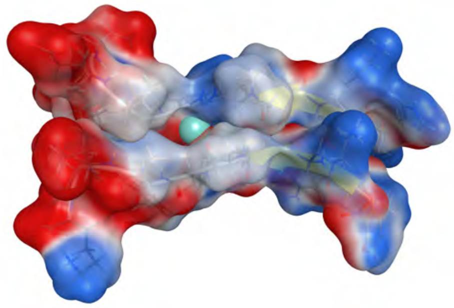
CECB Focus Areas

- Molecular recognition
- Organozymes, catalysis and processing
- GPCR's
- Proteolysis
- Protein "Click" chemistry and folding
- New chemistries for targeting disease

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.



At CECB we make combinatorial libraries of metal binding peptides that show activity in peptide hydrolysis.

Keywords

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

People

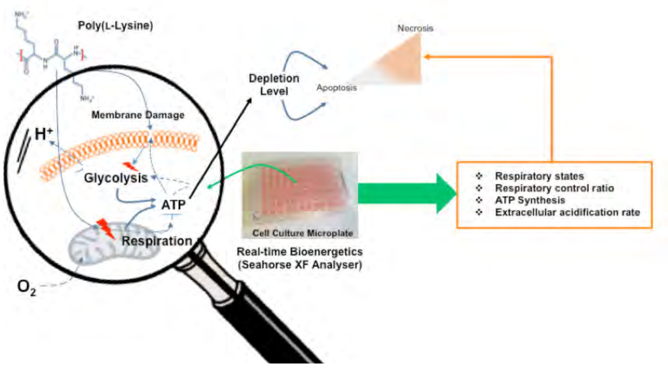
Prof. M. Meldal, Ass. Prof. F. Diness, 5 postdocs, 12 PhD students, 4 undergraduates

Contact

Prof Morten Meldal, +4521308299, meldal@nano.ku.dk

Centre for Pharmaceutical Nanotechonology and Nanotoxicology

We are engaged in tailor-made engineering of ‘safe-by-design’ and ‘safe-by-redesign’ of nanocarriers, functional nanomaterials and nanopharmaceuticals for site-specific targeting and biological engineering. The target sites include solid tumours (e.g. breast cancer), elements of the central nervous system (with particular emphasis on Alzheimer’s disease), lymphatic system and atherosclerotic plaques.



A pan-integrated metabolomic profiling for determination of polycation cytotoxicity mechanisms

Research Highlights 2015

- Comprehensive complement activation profiling and mechanistic insights of complement activation by graphene oxide, regulatory approved liposomal products, nucleic acid medicines, hexosomes and iron oxide nanoworms/nanocrystals.
- Demonstration of differential mechanical and immunological properties of tumour-derived exosomes dependent on malignant state.
- Immune-safe-by-design of hexosomes for drug delivery.
- Demonstration of therapeutic effect of engineered liposomes in transgenic mice models of human Alzheimer’s disease.

Personnel Achievements

- SM Moghimi: Co-organizer; Mechanisms and Barriers in Nanomedicine, Breckenbridge, CO, USA (will be held in June 2016).
- SM Moghimi Symposium co-chair, Nanoscience, Nanomedicine and Beyond: From Basic Science to Translation, University of Colorado Anschutz Medical Campus, CO, USA.
- SM Moghimi Appointed external supervisory board member (2015-2018), Horizon 2020 Marie Curie Actions-ITN Programme on ‘Design and development of advanced nanomedicines to overcome biological barriers and to treat severe diseases; NABBA’, University of Milano-Bicocca, Milan (Italy).
- SM Moghimi Visiting professor; Università Degli Studi Di Padova, Padova (Italy).

Current Funding

- CosmoPHOS-Nano: EU-FP7-NMP-LARGE (EUR 8.5 million; share of EUR 450,000)
- CAMNOT: The Danish Council for Independent Research, Technology and Production (DKK 5 million)
- NANOLYMPH: (with Dr. Anan Yaghmur, Pharmacy), The Danish Council for Independent Research, Technology and Production (DKK 5.4 million)
- Brain Capillary Enothelial Cell-Specific Peptidic Nanoplatforms: Lundbeckfonden (DKK 2 million)

Keywords

Advanced drug delivery systems, anaphylaxis, brain delivery systems, nanomedicine, nanotoxicology, nucleic acid delivery, nanopharmaceuticals

Selected Publications

[1] PP Wibroe et al., ***J Control Rel*** (2016) 221: 1-8 (with cover story by Kinam Park (Editor-in-Chief): J Control Rel 221, 76).
[2] S Inturi et al., ***ACS Nano*** (2015) 9: 10758-10768.
[3] B Whitehead et al., ***J Extracell Vesicles*** (2015) 4: 29685 – http://dx.doi.org/10.3402/jev.v4.29685.
[4] Hall, ***Biomacromolecules (American Chemical Society)*** (2015) 16: 2119-2126.

People

Prof. SM Moghimi; 5 PhD students; 4 postdocs; 3 visiting scientists.

Contact

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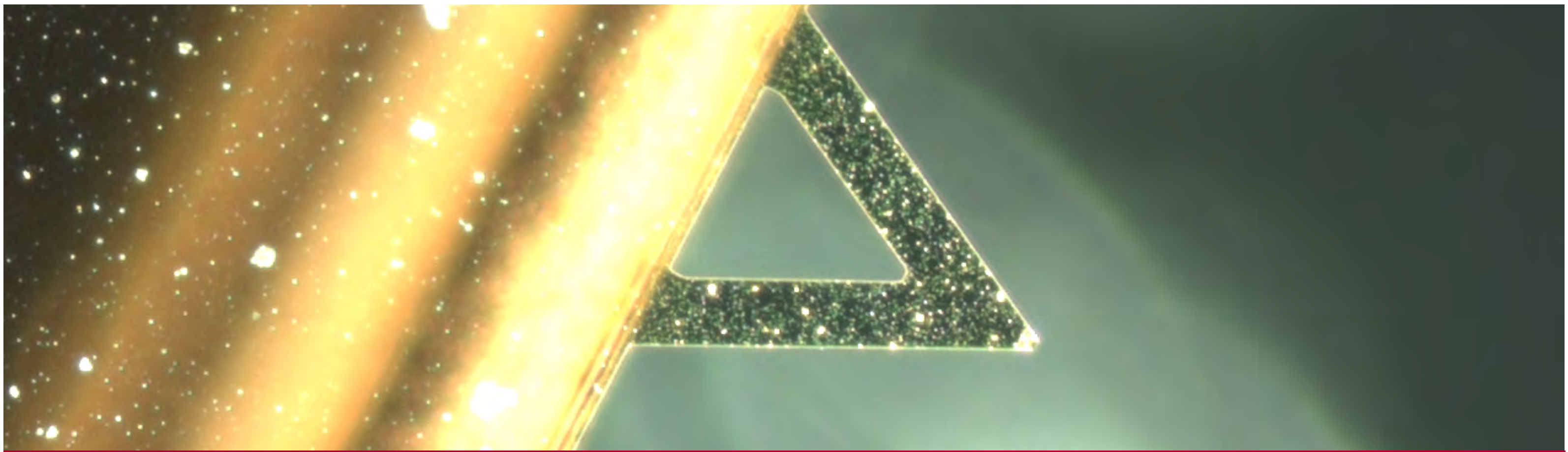

Condensed Matter Theory

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.

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.

Contact

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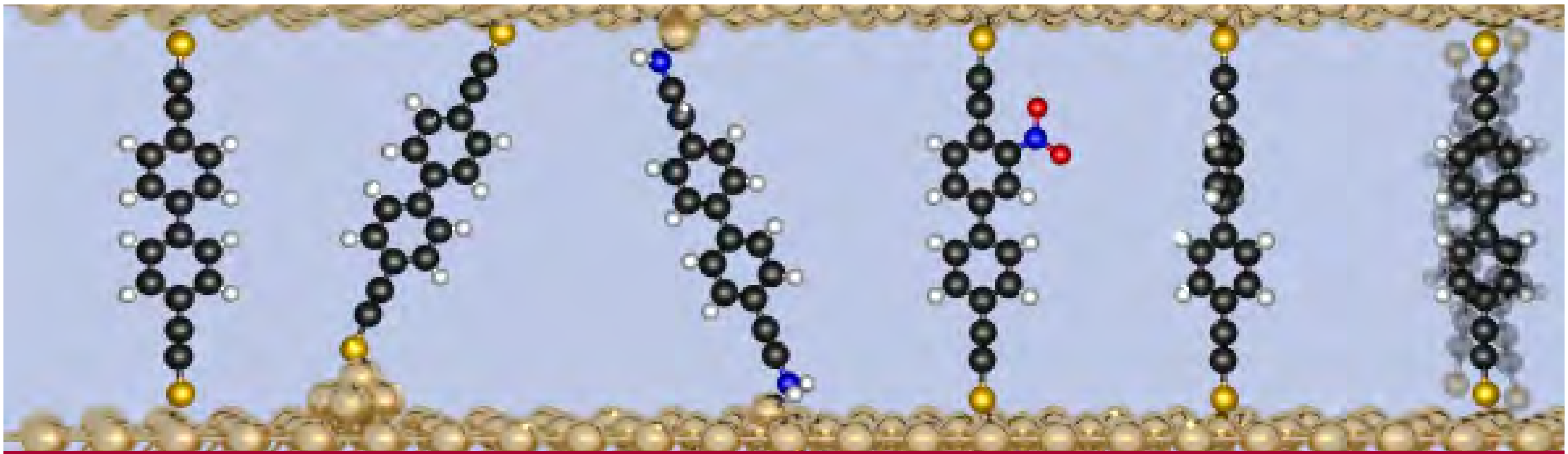


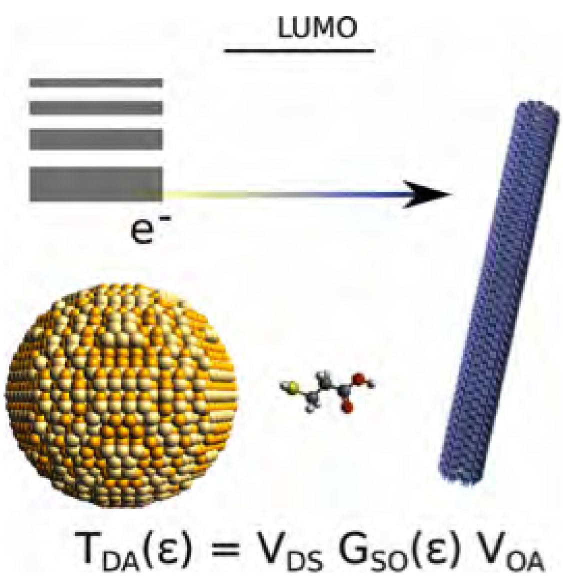
Molecular Electronics Theory

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.

The majority of the effort in the Solomon group was connected to the ERC project CHEMHEAT where we have continued with studies of the inelastic electron transport and heat transport in molecules. Qian Li defended her PhD thesis on her work.

The Solomon group also has a second major project "Simulating Single-Molecule Pulling Experiments" under a Sapere Aude grant. Three PhD students are working on the project and the first results on simulating the pulling of single-atom thick gold wires and hydrogen bonded complexes look very promising.

Gemma Solomon has also continued to have fruitful collaborations both within the University of Copenhagen and external partners. In July, she hosted a network meeting with participation of Nobel Prize recipient Roald Hoffmann.



The Hansen group focuses on its major project "Charge Transfer and Catalysis in Metalloproteins" funded by the Lundbeck Foundation. With collaborators in Lund, Sweden, Thorsten The Hansen group focuses on its major project "Charge Transfer and Catalysis in Metalloproteins" funded by the Lundbeck Foundation. With collaborators in Lund, Sweden, Thorsten Hansen continues 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.

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
2 postdocs	1 postdoc
5 PhD students	2 PhD students
1 Master's student	

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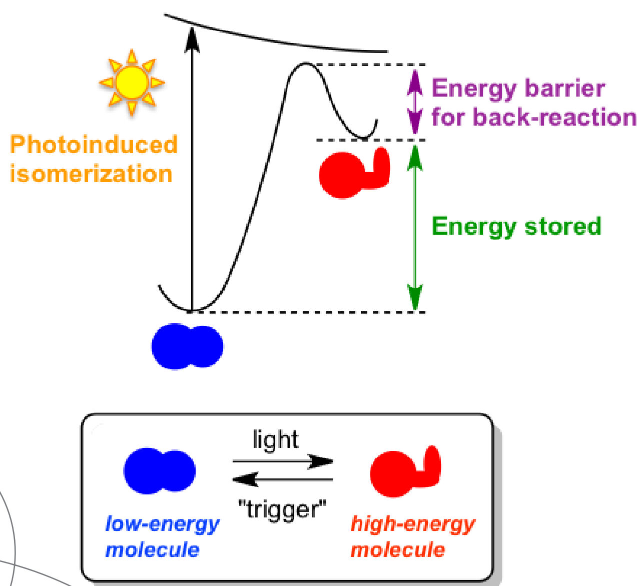
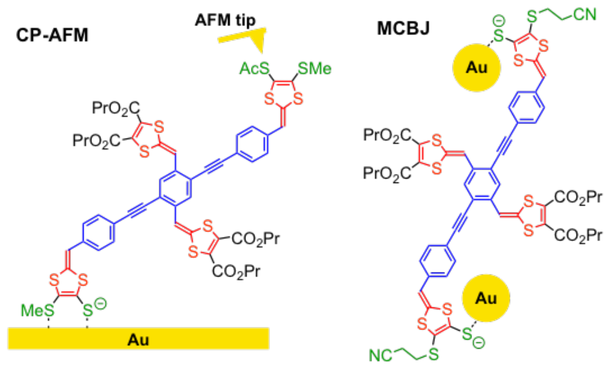
Molecular Engineering

The Molecular Engineering Group seeks to design, synthesize, and study functional macromolecules, in particular -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

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 redox-active tetrathiafulvalene and dithiafulvalene units.





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.

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.

Degrees

MSc degrees: Huixin Jiang, Mads Mansø, Martin D. Kilde, Frederik P. Jørgensen & Henrik Gotfredsen

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).

Contact

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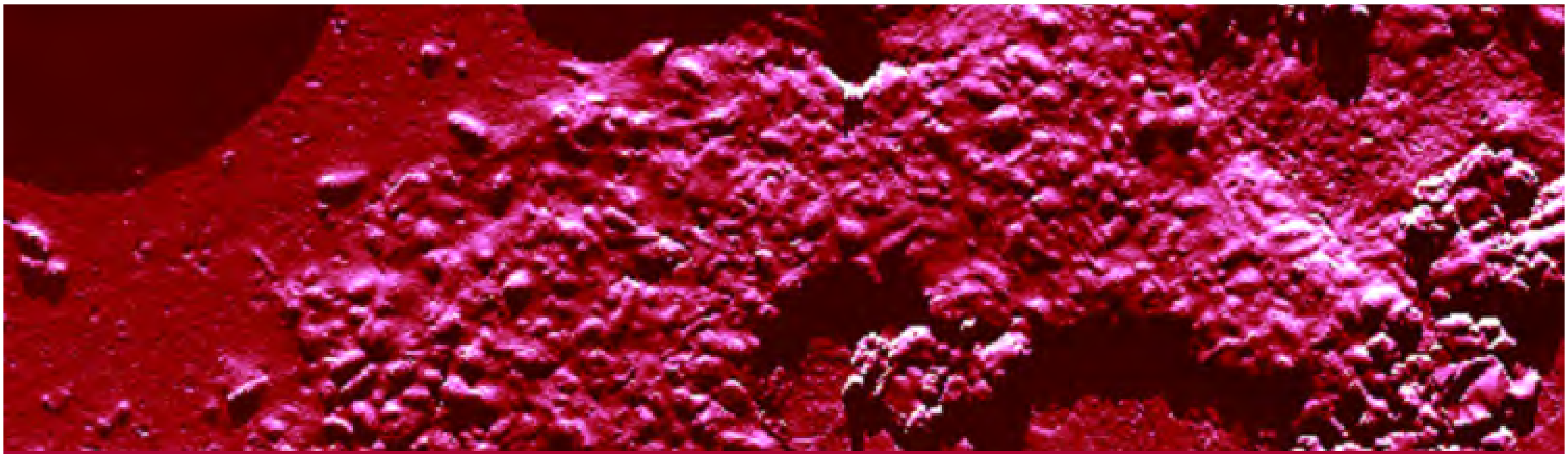
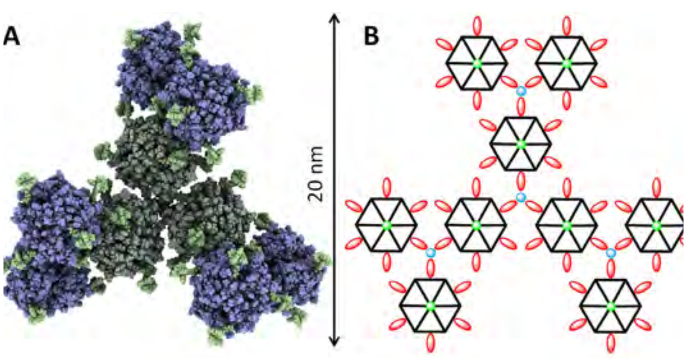


Nanobioorganic Chemistry

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.

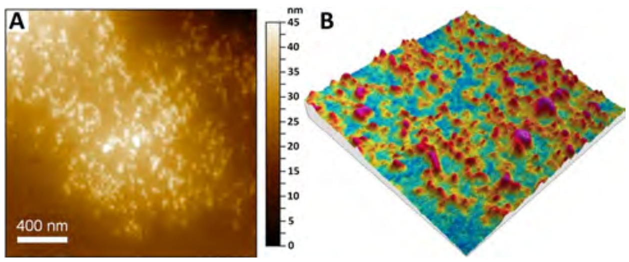
We seek to define and exploit the laws governing self-assembly of biomolecules in order to build biological meaningful nano-scale structures. The aim is to understand and control the self-assembly of biomolecules in solution and on surfaces. The ability to make defined nano-scale structures of biomolecules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

Organic synthesis is a powerful tool for the design and preparation of new materials on the Ångstrøm 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.



AFM image of self-assembled bipyridine-insulin

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.



Skematic representation of an bipyridine-insulin 54-mer.

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]Kawaharada Y., et al., ***Nature***, 2015, 523 (7560), 308-12.
[2]Leila Malik, et al., ***ChemBioChem***, 2015, 16 (13), 1905-1918
[3]Henrik K. Munch, et al., ***Angewandte Chemie Int.***, Ed. 2016, 10.1002/anie.201509088.

People

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

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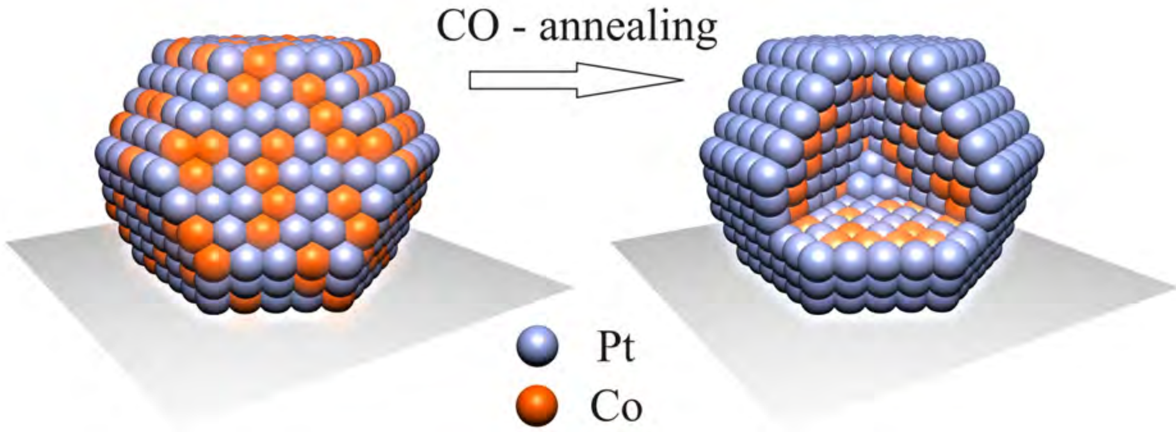


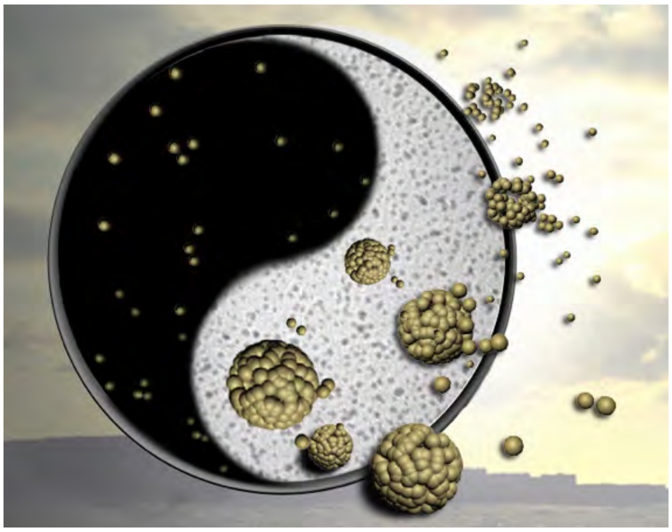
Nano Catalysis

Our research group is an international team devoted to the development of efficient and affordable electrocatalysts for sustainable energy conversion.
Through basic research we develop efficient and affordable hydrogen generation (electrolysis), and hydrogen conversion (fuel cells) systems. For the implementation of these technologies, the amount of the expensive Pt-based catalyst must be reduced and at the same time its durability increased.

Our research topics include
• synthesis and investigation of well-defined nanoclusters for energy conversion
• synthesis and investigation the activity and degradation mechanisms of carbon supported and unsupported electrocatalysts for PEM fuel cells
• novel concepts for cheaper and more durable catalysts
• influence of spectator-species in electrocatalysis
• develop improved electrochemical setups (soft- and hardware solutions) and procedures for catalyst testing.

In our research group we have several automated electrochemical test stands with RDEs and a multi-electrode setup. Our knowledge in this area led to the spin-out company Nordic Electrochemistry. We have one in-situ FTIR setup and one differential electrochemical mass spectrometry setup. Last but not least, we have equipment for catalyst synthesis. We frequently use TEM, SEM, and XRD at the Nano-Science Center.

At UCPH we work together with Assoc. Prof. J. Kirkensgaard concerning small X-ray scattering (SAXS), the research group of Assoc. Prof. T. Vosch concerning Raman Spectroscopy, and the research group of Prof. J. Rossmeisl concerning DFT calculations.
International collaborations include Prof. M. Baeumer and Dr. S. Kunz (Uni Bremen), Prof. U. Heiz (TU-Munich), and Dr. K. Mayrhofer (MPIE)
Furthermore, we collaborate with different groups within the 4M Center for Interdisciplinary Fundamental research to promote commercialization of HT-PEMFCs and the European DECORE consortium.
We are member of the Danish Electrochemical Society, the Danish Partnership for Hydrogen and Fuel Cells, as well as the Hydrogen and Fuel Cell Academy (HyFc).


Sketch illustrating the influence of light on the particle formation

Recent highlights of our research include the joint study with the groups of Tom Vosch and Sebastian Kunz concerning the influence of light on the particle formation in a colloidal synthesis of Pt Nanoparticles. The basic finding was that in a standard polyol synthesis performed at room temperature, the exposure to light is crucial for the particle formation process. This lead to the idea to use UV light to actively influence particle formation, an exciting new synthesis strategy for unprotected nanoparticles, which is currently under investigation.

Keywords
Electrocatalysts for low temperature fuel cells, stability of nanoparticles, catalytic properties of size selected nanoclusters, nanoparticles synthesis, and surface

People
Associate Professor Matthias Arenz, Dr. Alessandro Zana, Dr. Gustav Sievers, Michael Fleige, Yujia Deng, Anders Holten, Kaspar Holst-Olesen, Masanori Inaba, Bethan Davies, and Tim Sørensen.

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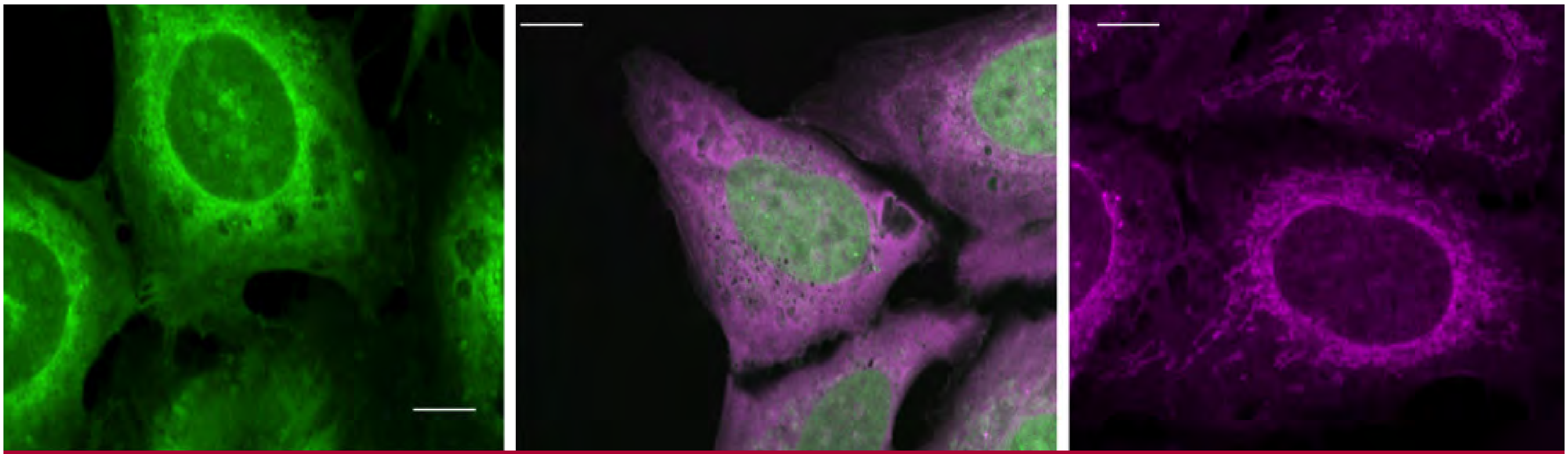


Nano Chemistry

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.

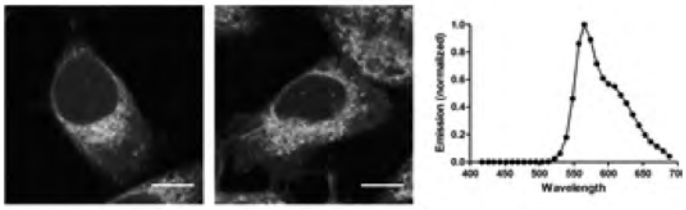
On the following two pages, you will find some examples of recent and on-going research in our group.

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***).

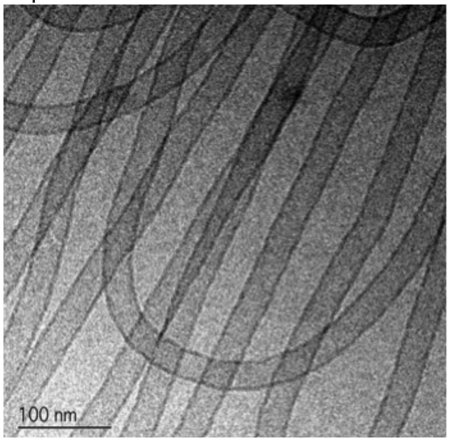
Detailed experimental and theoretical studies of the fundamental photophysical properties of pH sensitive rhodamine dyes have lead us to suggest a new model explaining the function of these important fluorescent indicators (***Chem Eur J 2015***).



Spectrally resolved fluorescence images of human cancer cells. We have been using a variety of our dyes to label cells; the figure shows where the dyes label the cells and the spectrum of recorded emission form the dyes.

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.



Cryo-TEM micrograph of 29 nm wide nanotubes self-assembled from amphiphilic cationic dyes in water (see ref 4 below).

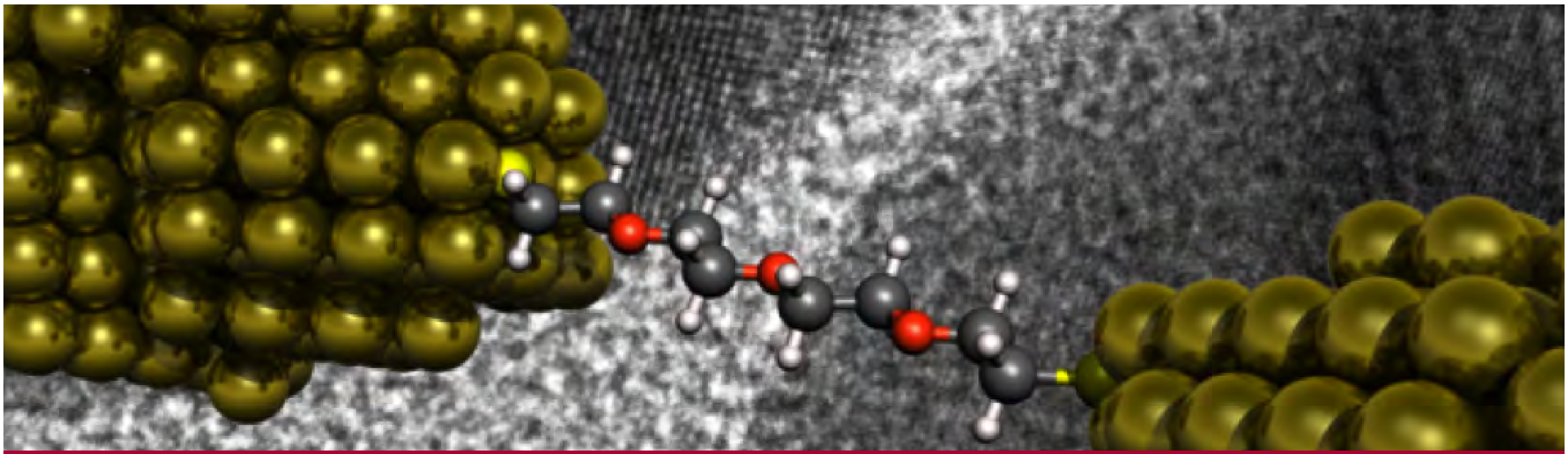
Selected publications

[1] Zhiyu et al, ***Chem. Comm.***, 2015, 51, 2372-2375

[2] Sørensen et al., ***Chem. Sci.***, 2015, 6, 2054-2059

[3] Sørensen et al., ***Chemistry – A European Journal***, 2015, 21, 8521-9.

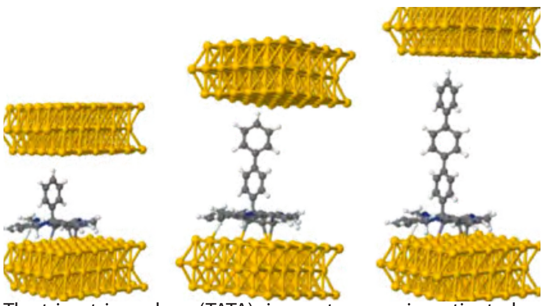
[4] Shi et al., ***Chemistry – A European Journal***, 2014, 20, 6853-6856



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. 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).



The triazatriangulene (TATA) ring system was investigated as a binding group for tunnel junctions of molecular wires on gold surfaces.

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 160 participants in 2015, will continue in 2016. carbonhagen.com

Keywords

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

Selected publications

[1] Wang et al., ***Nat. Commun.***, 2015, 6, Article number: 7478
[2] Wei et al., ***Langmuir***, 30, 2014, 14868–14876
[3] Jain et al., ***Acc. Chem. Res.***, 2014, 47, 2-11.
[4] Petersen et al., ***Chem. Mater.***, 2013, 25 (24), 4839–4848.

People

Professor Bo W. Laursen, Associate Professors Kasper Nørgaard and Thomas Just Sørensen, 4 postdocs, 6 PhD students, 8 undergraduates.

Contact

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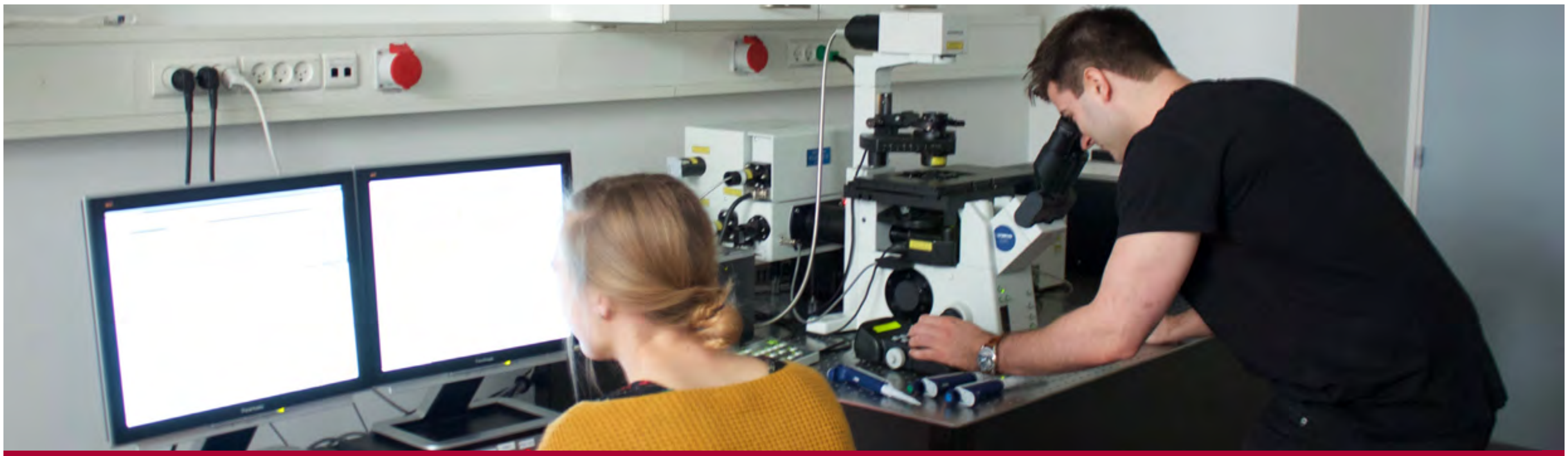


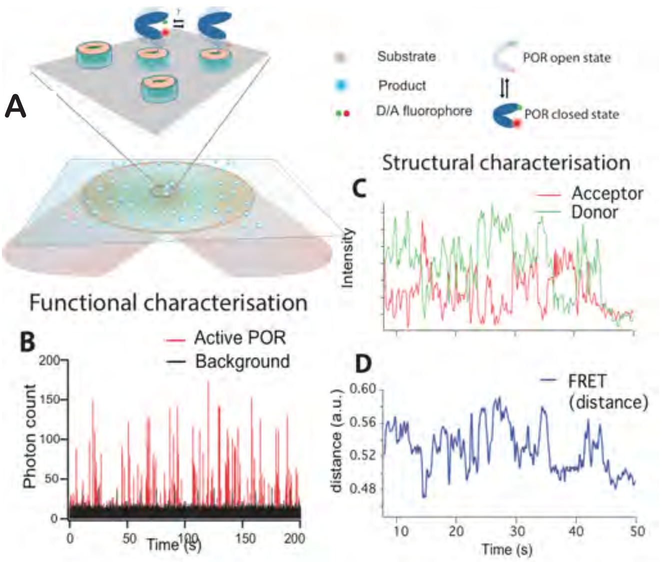
Nanoenzymology

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 chemistry, 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 single-molecule microscopes along with hiring new members.



A and B: Assay for immobilization of POR protein in nanodics for FRET analysis. C and D. Structural analysis of internal distances due to conformational changes in the POR protein using FRET efficenzy.

Selected publications

[1] M. Li et al., ***J. Am. Chem. Soc.***, 137, 16055-16063 (2015)
[2] S. Veshaguri et al., ***Science***, 351, 1469-1473 (2016).
[3] J. B. Larsen et al., **Nat. Chem. Biol.**, 11, 192-194 (2015).
[4] N. S. Hatzakis, ***Biophys. Chem.***, 186, 46-54 (2014).
[5] T. Laursen et al., **ACS Chem. Biol.**, 9, 630-634 (2014).

People

Nikos Hatzakis, Matias Moses, Stine Eiersholt, Darui Li, Camilla Thorlaksen, Simon Bo Jensen, Leonidas Lainis

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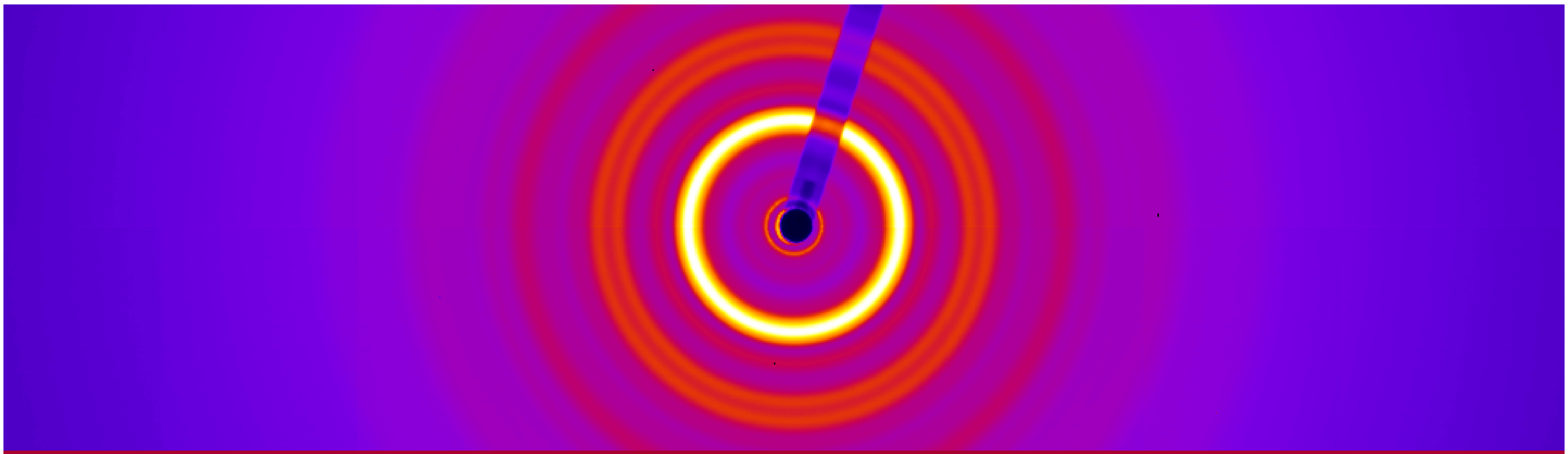


Nanomaterial Structure

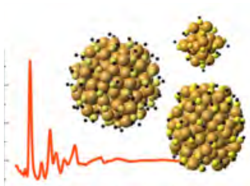
We are a new group at the Nano-Science Center and at UCPH, studying the synthesis and atomic structure in nanomaterials for energy conversion and storage. By means of advanced scattering techniques, we look into the arrangements of atoms in smart materials in an effort to map the relation between structure,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

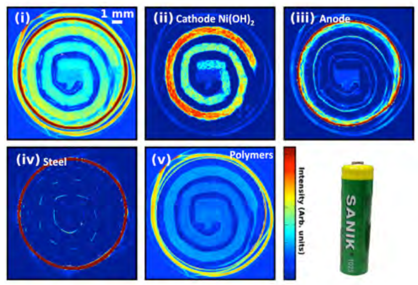
Nanomaterials by design

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. 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. magic sized noble metal nanoclusters as illustrated. 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. We are also involved in the development and use of ctPDF, a method for position resolved studies of nanostructure, which we have used to look into various devices and materials, e.g. batteries and catalysts.

'Magic-sized gold nanoclusters. By means of Pair Distribution Function analysis, we can elucidate the atomix arrangements in the clusters and relate this to the materials process.





Examples of ctPDF scans from a battery, allowing us to map the different phases in the battery.

News in 2015

We started our work at UCPH in October 2015, when Kirsten M. Ø. Jensen became assistant professor at Department of Chemistry. As a new group, we are building up our laboratory for nanomaterial synthesis, recruiting students and setting up for new research in nanostructure synthesis and characterization. Our research builds on KMØJ's previous work in materials chemistry and structure analysis. 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 several collaborations in both Europe and the US, we are part of the development of new methods for nanostructure characterization.

Keywords

Materials chemistry, nanoparticles, inorganic materials, materials structure, crystallography, X-ray scattering, neutron scattering.

Selected publications

[1] Kirsten M. Ø. Jensen, et al., ***ACS Nano***, 8, 10704-10714, 2014

[2] Kirsten M. Ø. Jensen, et al., ***J.Electrochem.Soc.***, 2015, 162, 7, A1310-A1314

[3] Kirsten M. Ø. Jensen, et al., ***IUCrJ***, 2015, 2, 481-489

[4] Sage Bauers, Suzzanah Wood, Kirsten M. Ø. Jensen, et al., ***J. Am. Chem. Soc.*** 2015, 137, 9652-9658

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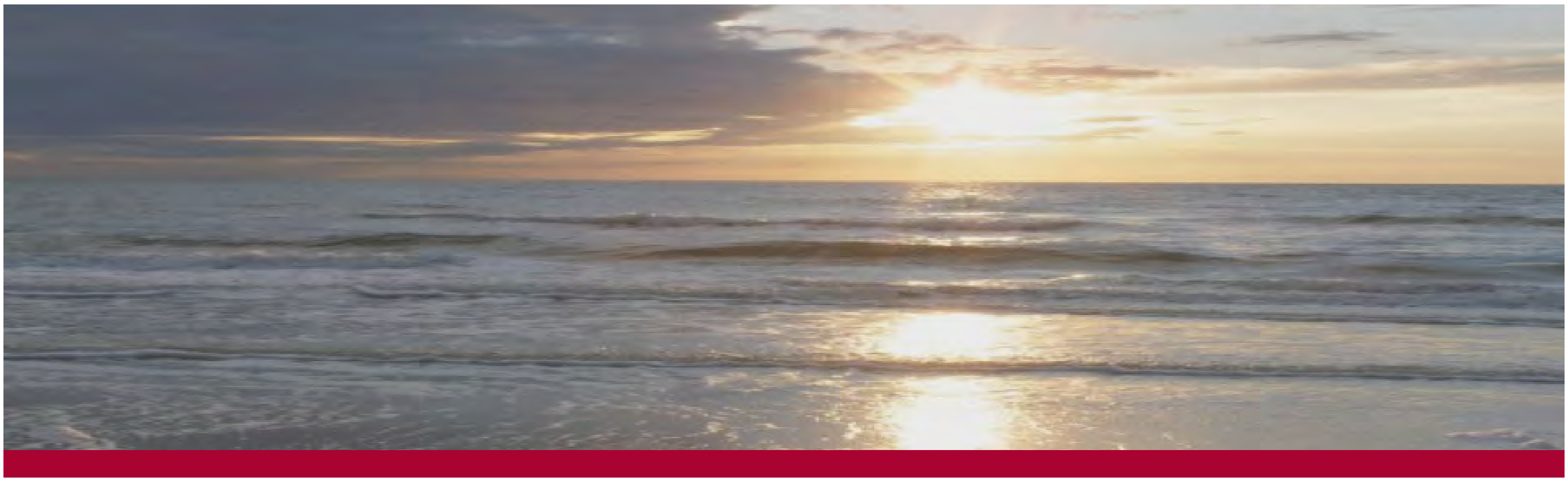


NanoGeoScience - Environment and Energy

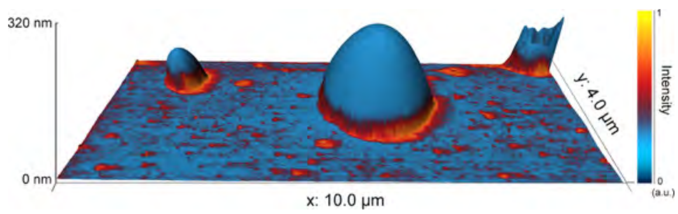
Nanotechniques let us “see” at the nanometre scale, where all the action is. We use them to learn nature’s secrets, to understand the fundamental physical and chemical processes that take place at the interface between natural materials and fluids (water, oil, CO_2, O_2, anything that flows). Then we 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 Danish Technical University and universities in Toulouse, F; Leeds, Warwick, University College London, York, Sheffield and Cambridge, UK; Oslo, N; Reykjavik, I; Karlsruhe, Münster, Potsdam and Max Planck Göttingen, D; Twente, NL; Waterloo, Canada; Berkeley and PNNL, USA as well as with several companies, including Maersk Oil, BP, DONG, Reykjavik Energy, Rockwool, Haldor Topsøe, Níras, COWI, GEO as well as AMPHOS21, a consulting engineering firm in Spain.

We have collected 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).

This year, we commissioned a new instrument, a NanoIR2. It is based on atomic force microscopy (AFM), which maps topography on surfaces with nanometre resolution laterally and sub-nanometre resolution perpendicular to the surface. Coupled to the AFM is a pulsed, tuneable infrared (IR) laser. Material on the 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 at that specific wavelength, e.g. 1,400 cm-1, representing C-O stretching and O-H bending (see figure below). We are excited about the possibilities for applying this capability in several current and future projects.



Aspartic acid on gold, analysed by infrared nanospectro-scopy. The 3D view is a superposition of IR and topography data. The electric field between the gold substrate and cantilever is enhanced, amplifying the IR signal in the 60 nm thick interface between the organic molecules and the substrate (red to yellow patches) (Hassenkam, Generosi et al., work in progress).

X-ray tomography (XCT) provides 3D images of the micro and nanostructure 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 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. There are also other interesting applications. For example, we worked with the Smithsonian Institute, USA to study biodegradation of handmade paper from the 17th century. XCT had not previously been applied on cultural heritage materials suffering fungal deterioration. This was a challenge because both paper fibres and fungal cells are made of organic compounds so X-ray attenuation for these materials is quite similar.

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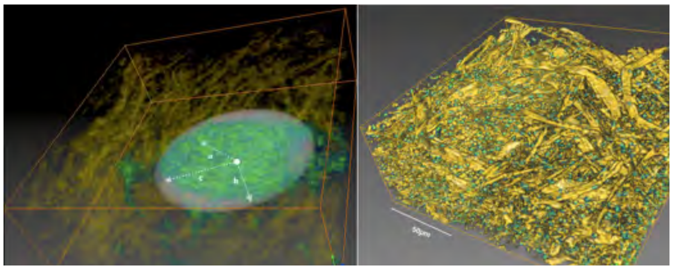
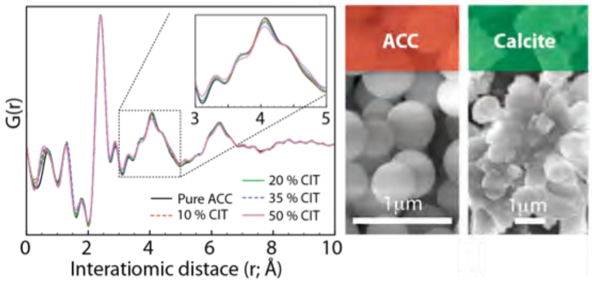
We developed a method to screen for shape, size and texture of the subspherical fungi to differentiate them from the cellulose fibres, which were larger and mostly linear. The 3D images showed that fungus permeated the paper, meaning that surface fungicide treatment can never be effective.



3D tomograms from 17th century paper. The subspherical bodies (coloured green) are fungus spores and the elongated fibres (yellow) are cellulose (Szczepanowska et al., 2015).

Some organisms use minerals for protection or support. They engineer organic molecules to enhance crystal growth with a form that fits their purpose. Understanding how CaCO3 transforms from the precursor, amorphous calcium carbonate ,ACC, to calcite or aragonite, in the presence of biomolecules, provides clues about the controls that organisms exert on their environment. Citrate is thought to modify local atomic structure in ACC, directing its transformation. Our analyses with microscopy, spectroscopy and advanced synchrotron X-ray scattering demonstrated that citrate dramatically enhanced ACC lifetime, thermal stability and changed calcite morphology but regardless of the concentration, the inter-atomic distances were minimally affected.



Interatomic distance for ACC with citrate (Tobler et al. 2015).

Funding
European Commission for Science, Innovationsfonden, Danish Research Council, Maersk Oil, BP, the Engineering and Physical Sciences Research Council (EPSRC) of the UK, Rockwool and the Capital Region of Denmark (Region Hovedstaden).

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
We published 44 articles in 2015 and presented 65 talks and posters at conferences. A few representative papers include:

[1] E. Hilner, et al., ***Sci. Rep.*** 5, 2015, Art. 9933.
[2] P. R. Mahaffy, et al., ***Science*** 347, 2015, 412-414.
[3] H. M. Szczepanowska, et al., ***J. Anal. At. Spectrom.*** 30, 2015, 651-657.
[4] D. Müter, et al., ***J. Phys. Chem. C*** 119, 2015, 10329-10335.
[5] D. J. Tobler, et al., ***Adv. Funct. Mater*** 25, 2015, 3081-3090.

People
Profs S. Stipp (Section Leader) and K. Bechgaard, Assoc. Profs T. Hassenkam, H.O. Sørensen, N. Bovet, M.P. Andersson, K.N. Dalby, D.J. Tobler, L. Lakshtanov; 7 assistant professors; 7 research, technical and admin. associates and assistants; 14 postdocs; 15 PhD students, 9 master's and 3 bachelor students; 2 guest researchers.

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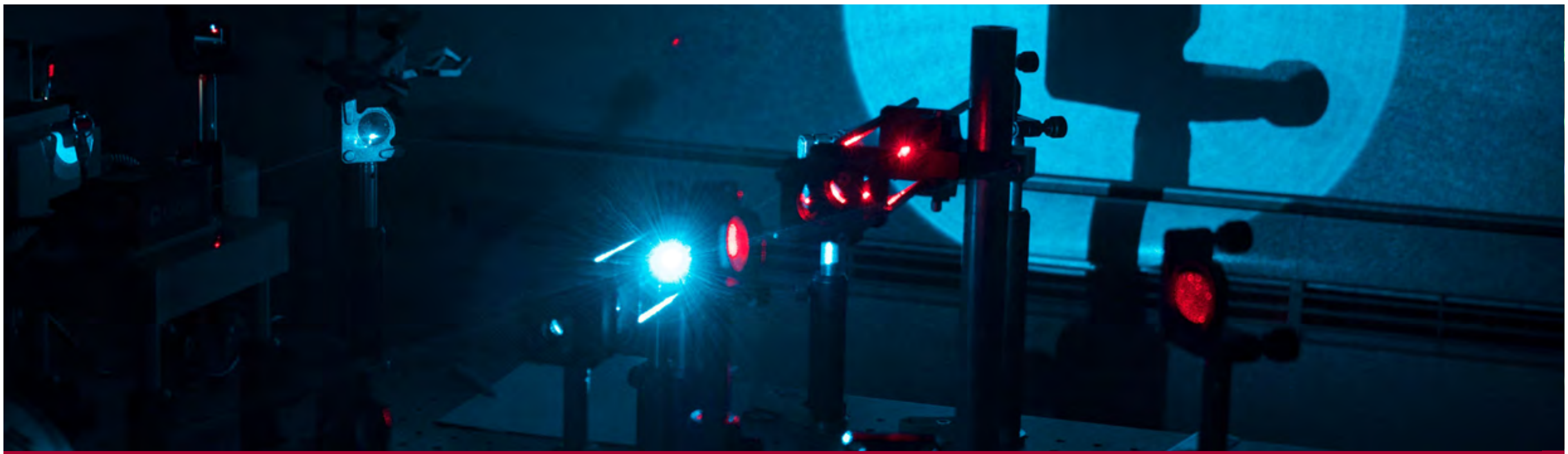


NanoSpectroscopy

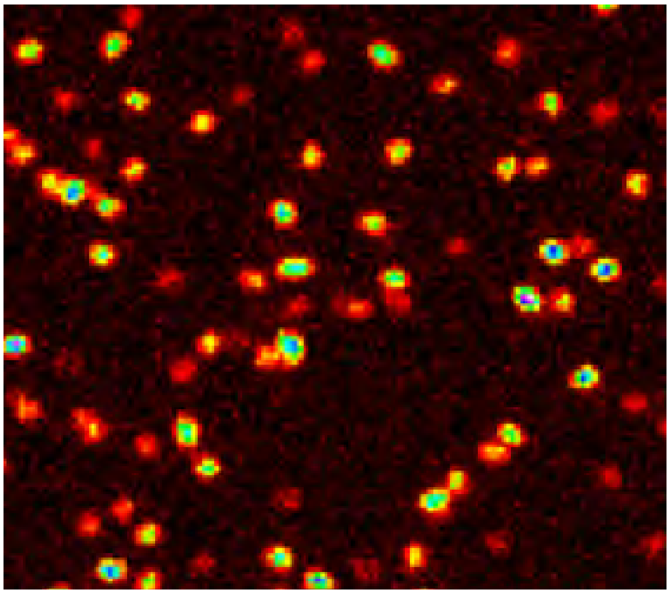
Our research group has a strong focus on studying the fluorescence properties of individual fluorophores by combining spectroscopy with microscopy. Single-molecule spectroscopy is a multidisciplinary technique, which has found many applications in the field of material and life science characterization.

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, Lanthanide microscopy and silver nanoclusters.



An example of a confocal fluorescence image showing a number of well separated individual molecules (image size: 20 by 20 micron).

Keywords

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

Selected publications

[1] Liao; Hooley et al., ***J. AM. Chem. Soc.***, 2013, 135, 19180-19185.

[2] Hutchison; Uji-i et al., ***Nat. Nanotechnol.***, 2014, 9, 131-136.

[3] Hooley; Paolucci et al., ***Adv. Opt. Mat.***, 2015, 3, 1109-1115.

People

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

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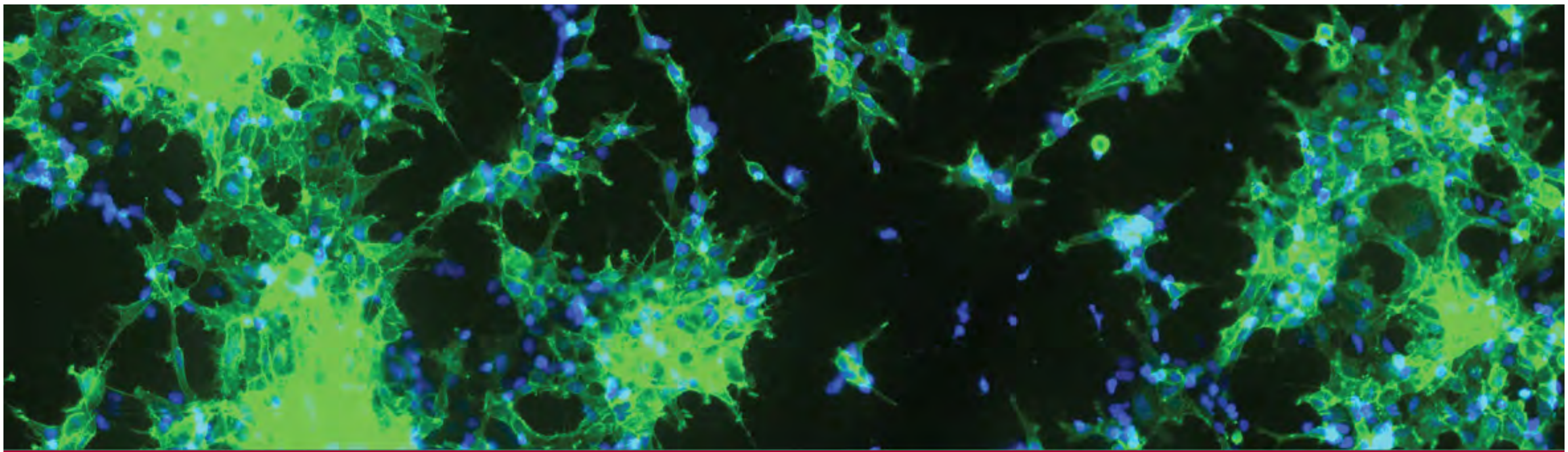

Quantum Devices

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.

Highlights from 2015

- Center reached a staff of more than 70 researchers, incl. professors, postdocs, PhDs and students
- QDev and QuTech (Technical University of Delft) established a Scientific Exchange Program, which was initiated with a Memorandum of Understanding ceremony at the Danish Parliament with Prime Minister Helle Thorning-Schmidt and the Dutch royal couple, King Willem-Alexander and Queen Máxima
- QDev had over 142 Danish and international visitors and hosted 35 seminars and lectures.
- QDev physicist Jessica Bolinsson received a grant from the Villum Foundation's Young Investigator Programme.
- QDev physicist Fabrizio Nichele received a grant from the EU Marie Curie Fellows Program
- QDev physicist Mark Rudner received ERC grant of nearly 12 million kroner
- QDev research article by Larsen et al. on a new qubit scheme was featured as Editor's Choice in Science Magazine
- QDev researchers are behind the breakthrough on a new type of 'nanowire' crystal that fuses semiconducting and metallic materials on the atomic scale lay the foundation for future semiconducting electronics.
- Two independent groups have now demonstrated a new qubit scheme, consisting of two superconductors bridged by a nanowire, that could help researchers design quantum circuits with more flexibility. The teams, led by Leonardo DiCarlo at Delft University of Technology in the Netherlands and Charles Marcus at the University of Copenhagen in Denmark, have demonstrated structures in which the nanowire replaces one of the basic elements of a superconducting qubit—the insulating barrier between two superconductors that forms a Josephson junction.

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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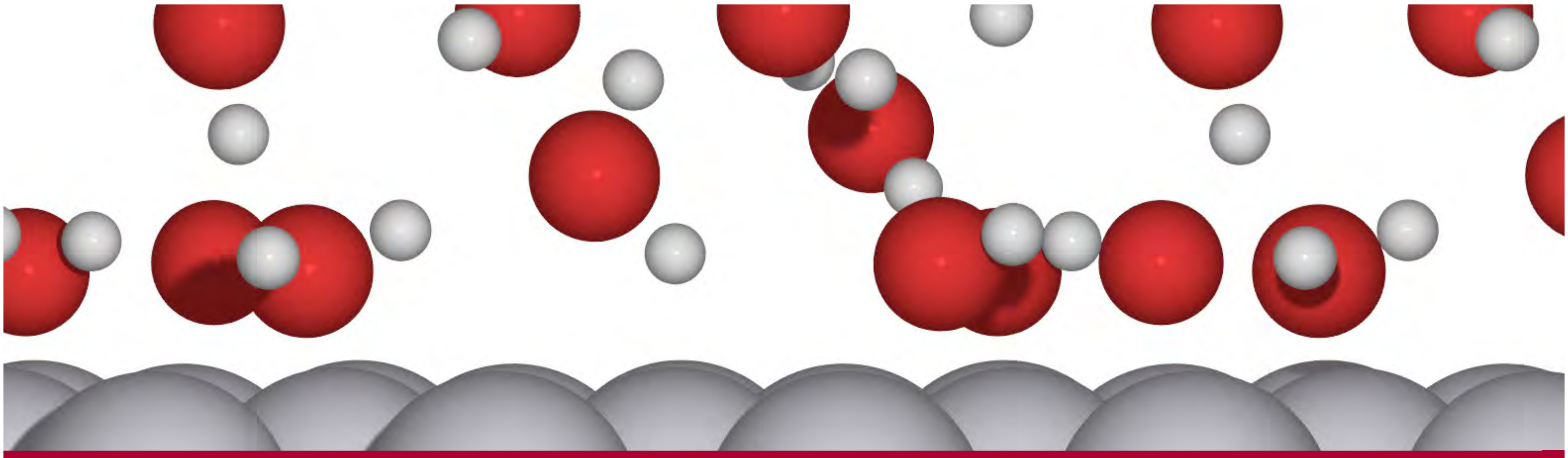
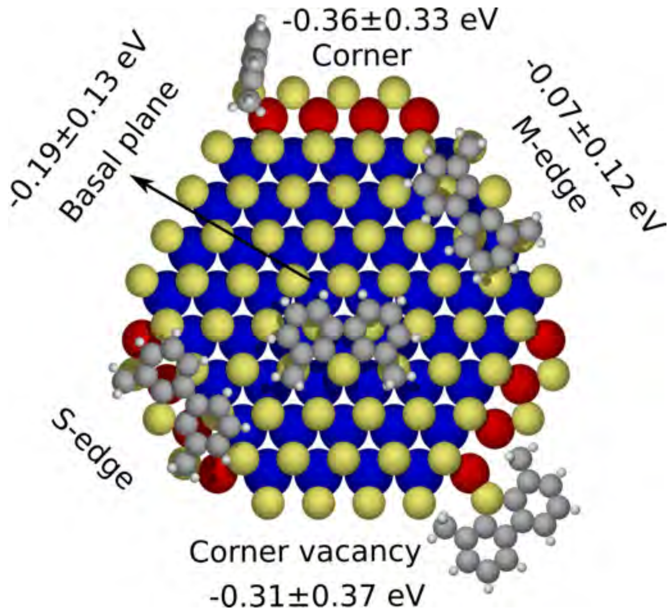


Theoretical Electrocatalysis

The group was established at the UCPH Department of Chemistry and joined the Nano-Science Center in April 2015. 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.



Atomic-scale model of desulfurization catalyst.

Highlights from 2015

• Jan Rossmeisl was appointed professor.
• The supercomputer cluster "Katla" (Short for Katalysis Lab and the name of a volcano) was setup and running.
• In November, the group received DKK 500,000 from Carlsbergfondet for expanding Katla.
• A research project funded by BMW was initiated and a KIC project was funded.
• The first PhD students, master's and bachelor students have started in the group.

Keywords

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

Selected Publications

[1] M Bjorketun Nielsen et al., ***Surf. Sci.***, 631, 2-7, 2015 DOI: 10.1016/j.susc.2014.08.018
[2] R. Frydendal et al., ***ChemCatChem*** 7, 149-154, 2015 DOI: 10.1002/cctc.201402756
[3] MH. Hansen; Stern et al., ***Phys. Chem. Chem. Phys.***, 17, 10823-10829, 2015 DOI: 10.1039/c5cp01065a
[4] R. Frydendal et al., ***Adv. Energy Mater***, 5, 1500991, 2015, DOI: 10.1002/aenm.201500991
[5] V. Tripkovic et al., ***ACS Catal.***, 5, 6032-6040, 2015, DOI: 10.1021/acscatal.5b01254

People

Postdoc: Ivano Castelli
PhD students: Martin Hangaard Hansen, Manuel Saric, Thomas Østergaard, Alexander Bagger.

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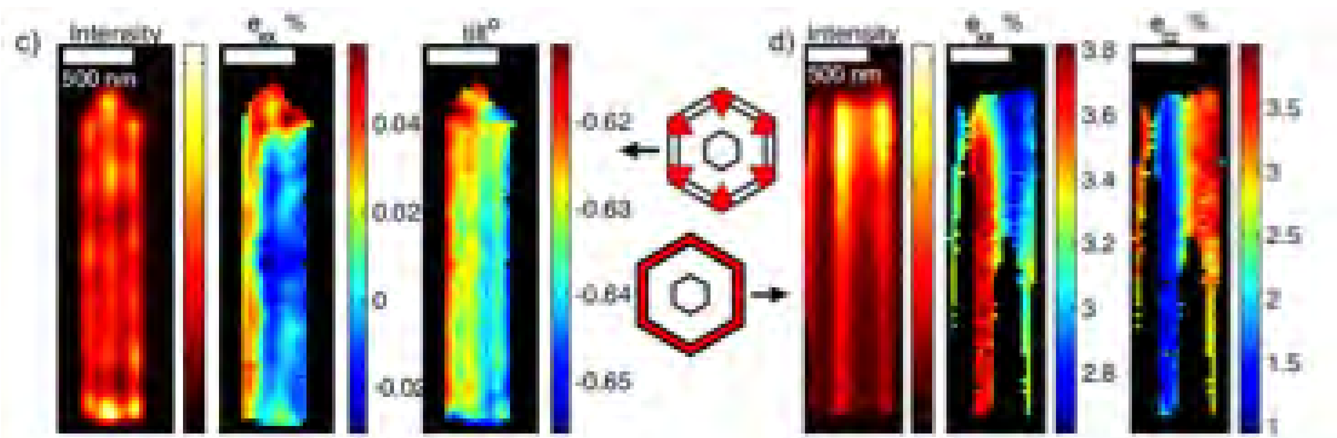

X-ray and Neutron Science

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 nanodisc is particularly central for structural investigations of membrane proteins.

Highlights from 2015

A number of studies rely on the controlled contrast for neutron scattering. Contrast variation is however also possible in X-ray scattering [1]. 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 [2]. Our group 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.

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 are ideal for such studies, and we have demonstrated that the development of nanoscale hydrogen-bonded network is the key to the performance of new "green materials" [5].

Apolipoprotein A1-based nanodiscs have emerged as a platform for studying membrane proteins [3]. We have developed a peptide system that mimics 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 [4].

Schematic illustration of artificial peptide nanodisc with embedded membrane protein

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 [5].

Keywords

X-ray and Neutron Science, including small-angle, elastic and inelastic scattering and imaging. Soft Matter, Biomolecules, Superconductivity and Magnetism. Experiments, Simulations, Theory and Instrumentation.

Selected publications

[1] K. Mortensen et al. , ***Colloid Polym. Sci.*** 293, 3353 (2015)
[2] K. Lefmann, et al. ***Phys. Rev.*** B 91, 094421 (2015)
[3] S.R. Midtgaard, et al. ***Biophys J***, 109, 308.(2015)
[4] A.R. Benetti et al., ***Sci. Rep***. 5, 8972 (2015).
[5] T. Stankevic, et al. ***ACS Nano*** 9, 6978 (2015).

People

K. Mortensen, R. Feidenhans'l, L. Arleth, K. Lefmann, B. M.Andersen, H. N. Bordallo, L. H. Øgendal, S. L. Hansen, L. Udby & J. Kirkensgaard. 6 postdocs and 25 PhD students.

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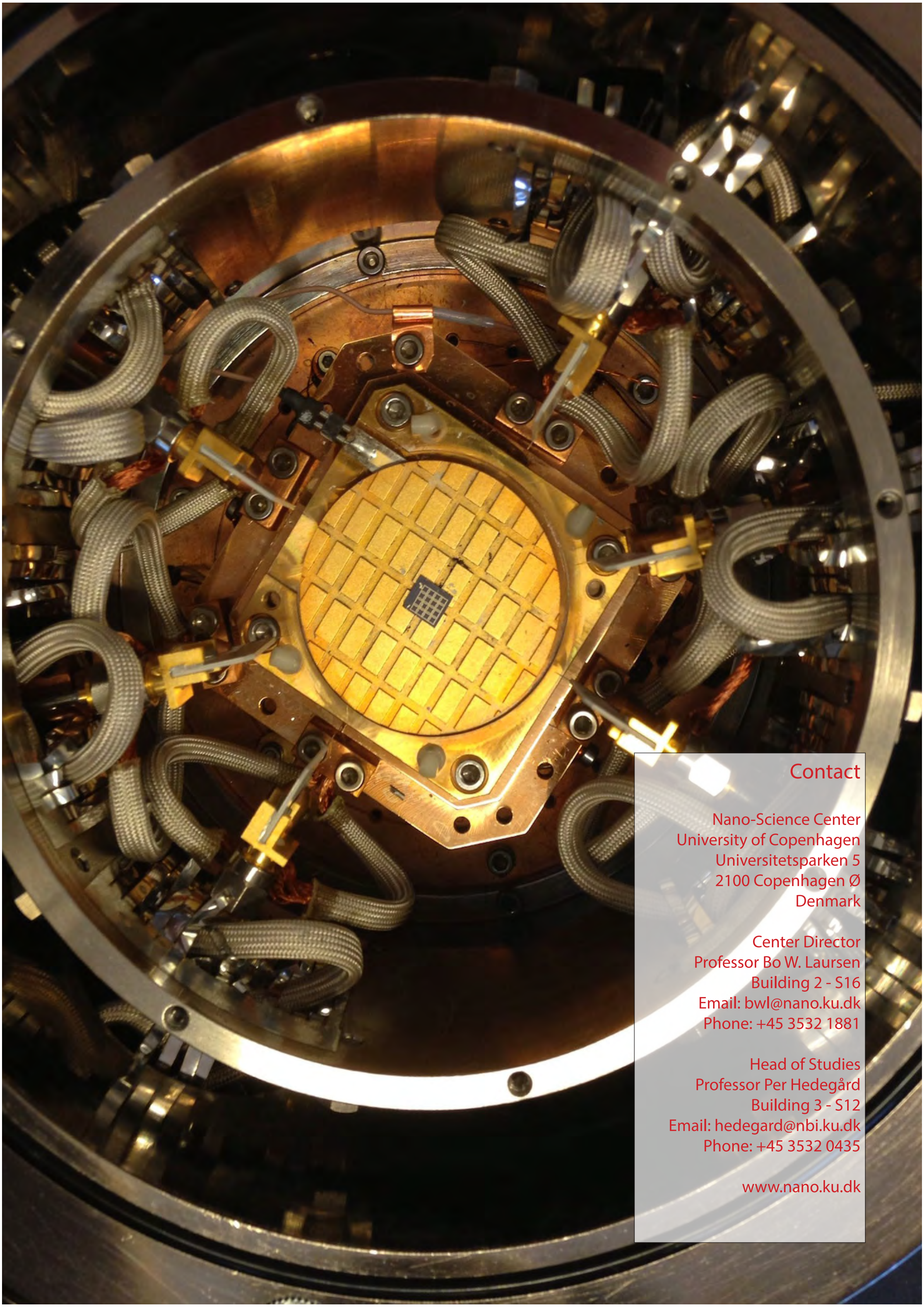

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