Department of Chemistry

DTU Chemistry 2021

Contents

Ramping up our influence on the green transition

Chemistry plays a crucial role in meeting the challenges of the green transition. We must continue to develop and fine-tune sustainable technologies, materials, and chemicals that enable us to live in a modern world while protecting our planet.

DTU Chemistry takes on key responsibilities that facilitate and drive the green transition. In 2021, we have, together with several other universities and industrial partners, provided roadmaps within the national so-called Innomissions. The roadmaps define common directions for research and innovation that will lead to significant CO_2 reductions on both short and long term.

As you can read in this booklet, our researchers have an innovative approach to both basic research and in the development of, e.g., materials and medicines with great application potential. This year new ambitious proposals have led to a total of 93 MDKK in additional external funding – a departmental record.

In 2021, 14 PhD students graduated and 23 were enrolled. Our research groups benefit vastly from the

Head of Department, Erling H. Stenby.

curiosity and dedication of our PhD students, and we are pleased to experience an increasing interest by industry and academic partners to join forces and form collaborations.

We look forward to continuing the consolidation of DTU Chemistry as a strong partner and driver of the green transition through research, innovation, and education.

Head of Department,
Erling H. Stenby

Two major research sections

The research sections of DTU Chemistry contribute through different methods to new knowledge and solutions in areas such as new medicine, clean energy technologies, and new sustainable materials for the benefit of people and environment.

Organic and Inorganic Chemistry

This section is developing effective compounds by comprising activities within catalysis and sustainable chemistry, materials chemistry, and organic chemistry.

Common themes are the synthesis and characterization of small to very large inorganic and organic molecules.

Research areas are homogenous and heterogeneous catalysis; gas separation and absorption; development of new materials; conversion of biomass; electrochemistry; new synthetic methods; coordination chemistry; chemical biology; NMR spectroscopy.

Physical and Biophysical Chemistry

This section comprises activities within pure and applied physical chemistry. It covers both microscopic atomic-level descriptions and the macroscopic thermodynamic approach.

Common themes are determination of structure and behaviour of small to medium-sized molecules as well as proteins, and many projects involve spectroscopy, scattering, and computer modelling.

Research areas are biophysical and biomedicinal chemistry; high pressure phase behaviour for petroleum processing and CO2 sequestration; polymers and functional interfaces; IR and THz spectroscopy; theoretical, computational, and femtochemistry.

Research in figures

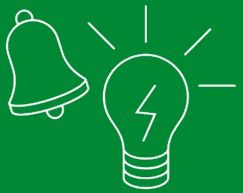
181
Publications in 2021
WoS-indexed journals

27 faculty
21 postdocs
5 researchers and
senior researchers

1.19
Normalized citation impact

13.4%
Publications in top 10%

28
BEng, BSc, and MSc projects
completed with industry



42
WoS publications in
cooperation with industry

93 MDKK
in external funding

Funding


Photo: Morten Larsen, DFF

Associate Professor awarded ERC Starting grant and named Sapere Aude Research Leader

Associate Professor Sophie Bereen received a prestigous starting grant from the European Research Council (ERC) of just over 11 MDKK.

Her project '*ENZYME-DCC*' will explore a conceptually new approach to using enzymes for chemical synthesis that combines tools and concepts from synthetic chemistry with enzymology. In this new methodology, enzymes catalyze reversible reactions and generate complex dynamic mixtures of interconverting products. So-called template molecules are then added to recognize and select desired products from the mixtures.

In nature, biomolecular templates define the outcomes of enzymatic reactions in some of the most fundamental biological processes, such as DNA replication, transcription and translation. This project investigates the possibility of using synthetic templates to direct enzymatic reactions and access different products to what is formed in nature.

Sophie Beeren was also awarded a 6.2 MDKK Sapere Aude Research Leader starting grant from the Independent Research Fund Denmark. The project '*Harnessing the Power of Dynamic Interconverting Glycans for Oligosaccharide Synthesis*' will explore a new way of using enzymes for the synthesis of oligosaccharides.

The research group will use enzymes to reversibly connect together monosaccharide building blocks and generate dynamic mixtures of different interconverting oligosaccharides. They will then use artificial template molecules that bind, stabilize and thus promote the selective synthesis of specific oligosaccharide products.

Hallas Møller Emerging Investigator will examine cholesterol transport with sterol mimicking compounds

Associate Professor Luca Laraia was awarded a Hallas Møller Emerging Investigator grant of MDKK 9.9 from the Novo Nordisk Foundation for his project '*Determining mechanisms of intracellular sterol transport with selective chemical probes*'.

To better understand the role of cholesterol transport proteins in health and disease, the project aims to develop molecules that can selectively block the function of any specific one, without affecting the others. For this, the project will use a collection of developed compounds which mimic sterols and are ideally suited for identifying new blockers of cholesterol transport proteins.

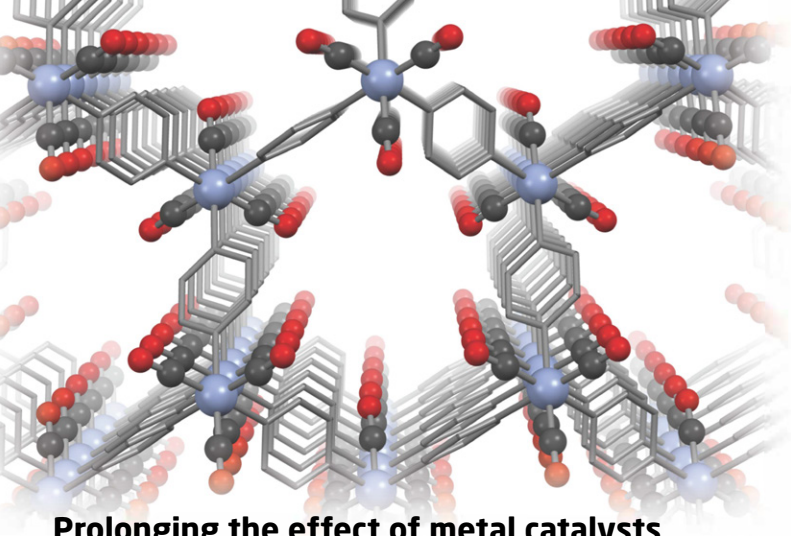
The goal is then to optimize these molecules to be selective and study their effect on cellular cholesterol transport and cancer cell proliferation.

Two projects fueled by Green Transition Grant

DTU Chemistry has received funding from Independent Research Fund Denmark (DFF) for two green research ideas. Both projects have high ambitions for exploiting energy sources in a more efficient way.

Associate Professor Martin Nielsen, DTU Chemistry, will – together with Professor Shoubhik Das from the University of Antwerp – develop a new method for transforming CO_2 into useful chemicals under mild conditions. The project '*Green CO_2 Transformations Using Synergistic Catalysis*' was granted approx. 5.6 MDKK.

The other recipient from DTU Chemistry is Professor Klaus B. Møller. He is co-recipient on the project '*Ultrafast Mapping of Singlet Fission for Solar Energy Conversion (UltraSol)*' with Professor Martin Meedom Nielsen, DTU Physics. The project - granted approx. 6.2 MDKK – will reveal the mechanisms behind solar-to-electric energy conversion in organic materials with a profound impact on solar cell design.



Prolonging the effect of metal catalysts

Zero-valent metal ion complexes are efficient catalysts for small molecules such as N_2, H_2, and CO_2. However, their high chemical reactivity in the activated state leads to side-reactions, decomposition, and loss of activity. Associate Professor Kasper Steen Pedersen has been granted approx. 5 MDKK by the Carlsberg Foundation for the development of a novel field on the chemistry of low-valent metal ion nodes immobilized in rigid frameworks. This will impede the disintegration of the active catalytic sites and thus provide perspective of developing a genuinely new generation of catalysts for small molecule activation and, in particular, CO_2 reduction.

Investigating underground reservoirs for CO_2 storage

Project Greensand is maturing one of the most progressed carbon capture and storage (CCS) projects inside Danish jurisdiction and targets the development of CO_2 storage capacity in the Danish part of the North Sea based on reusing discontinued offshore oil and gas fields for permanent CO_2 storage.

The Phase 2 of the project received 197 MDKK in total from the Energy Technology Development and Demonstration Program (EUDP) via the Danish Energy Agency. As part of the project, Associate Professor Wei Yan from DTU Chemistry received 3.9 MDKK to investigate what happens if a huge amount of CO_2 is injected into the underground storage site currently filled with brine and residual oil.

Developing a 3D printer based on light dose distribution

Assistant Professor Yi Yang from DTU Chemistry has been awarded a Villum Experiment grant of 2 MDKK for developing an ultra-fast, revolutionary 3D printer.

"Our printer will build a physical object at the intersects of computed tomographic images. The technology enables us to build 3D objects embedded with different properties and material transitions. The printing takes place instantly and with great precision because the process is only light-dependent," says Assistant Professor Yi Yang".

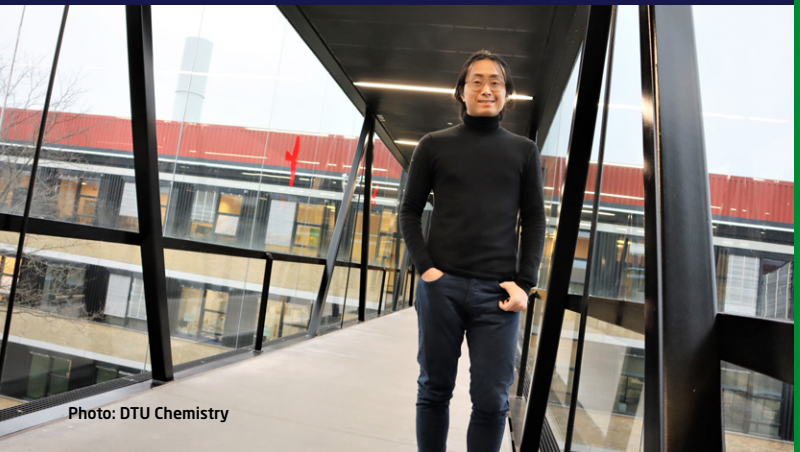


Photo: DTU Chemistry

Other notable funding

Independent Research Fund Denmark

- Anders Riisager, '*Sustainable Aviation Fuel from CO_2 by Combined Fermentation and Catalytic Conversion'*, 3.2 MDKK
- Mads Hartvig Clausen and Charlotte Held Gotfredsen, *'Selective Small-Molecule Probes for TNF Receptors'*, 3.1 MDKK
- Katrine Qvortrup, ' *Selective delivery of drugs to CNS for treatment of neurological diseases'*, 2.6 MDKK

The Novo Nordisk Foundation - NNF Project Grant Nat.Tech

- Anders Riisager, '*Valorization of CO_2 to ethanol with benign cascade catalysis'*, 3 MDKK
- Søren Kramer, ' *Photocatalysis for Medicinal Chemistry'*, 3 MDKK

The Novo Nordisk Foundation - Expl. Int.disc. Synergy Grant

Katrine Qvortrup, '*Tailored Drug Access to CNS: An Interdisciplinary Study Exploring Solutions for Improved Treatment'*, 1.5 MDKK

Lundbeck Foundation

Cecilia Romanó, *'iNKT cell-based cancer immunotherapy – a synthetic toolbox for developing novel cancer vaccines'*, 1.6 MDKK

Sygeforsikring Danmark

Katrine Qvortrup, '*High-potency solution against bacterial biofilms - expanding the global arsenal against antibiotic resistance'*, 1.4 MDKK

EU - MSCA-IF

Bruno Nunes Cabral Tenorio, ' *Theoretical beamlines to time-resolved ultrafast Auger electron spectroscopy (TR-AES)'*, 1.6 MDKK

Two new Villum Young Investigators

Early 2021, two Assistant Professors joined the Department. Both researchers have been awarded a Villum Young Investigator grant and strengthen the research area of computational chemistry.

Janus Juul Eriksen

Villum Young Investigator (2021):

DECODENSE: Mean-Field Density Matrix Decompositions

Computer simulations nowadays find use in unravelling the inner workings of, e.g., potential drug propects or emerging solid-state batteries, particularly whenever traditional empirical explorations prove infeasible. To that end, this project is concerned with the acceleration of contemporary electronic structure methods by means of modern machine learning.

Jógvan Magnus Haugaard Olsen

Villum Young Investigator (2020):

Computational Spectroscopy of Biomolecular Systems

Spectroscopy is essential for furthering our understanding of the structure and function of biological material. However, the use of advanced spectroscopies is hampered by the difficulty of intepreting the results. This project aims to develop computational methodologies that can simulate a wide range of biomolecular spectroscopies and thus be used to interpret the outcome of experimental studies.

Developing a cancer vaccine

Professor Mads Hartvig Clausen and postdoc Cecilia Romanò from DTU Chemistry have succeeded in synthesizing the carbohydrates of cancer cells, which has enabled them to develop a vaccine candidate with potential to combat breast cancer, neuroblastoma (a type of tumour in children), and small cell lung cancer.

Collaborations across departments at DTU and scientific areas have been key during the process.

"As we began the project, we knew about the strong competencies within immunology and drug delivery there are at DTU. Our research group has expertise in chemical synthesis but sought expertise on the other things in order to succeed in developing the vaccine. Therefore, we formed collaborations with colleagues from DTU Healthtech and DTU Bioengineering," explains Mads Hartvig Clausen.

Testing of the vaccine in mice shows promising results.

Photo: Mikal Schlosser

Read the full article (in Danish) in DTU Dynamo

Selected publications

DTU Chemistry has a high performance in the world of chemical science. This is reflected in all the publications produced and published in high impact journals every year.

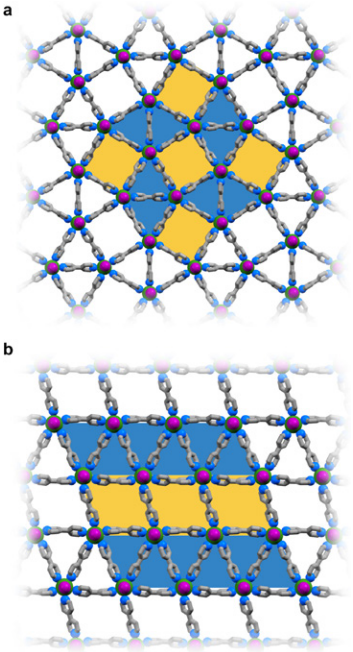
In the following pages, you can read some examples of the Department's exciting results and publications during 2021.

For a complete list scan the code or visit:

kemi.dtu.dk/english/aboutus/publications.

New recipe tiling 2D magnetic materials

Associate Professor Kasper Steen Pedersen and seven other DTU Chemistry colleagues report a recipe to tile 2D magnetic materials using molecular chemistry and lanthanides.



The implementation of Archimedean tessellations in lanthanide(III) coordination solids couriers a strategy to design elusive quasi-periodic metal-organic frameworks with inimitable magnetic properties.

Title: *Magnetic Archimedean Tessellations in Metal-Organic Frameworks*

Published in JACS as the inside cover
J. Am. Chem. Soc. DOI:10.1021/jacs.1c05057

Combating biofilm of multiresistant bacteria

Associate Professor Katrine Qvortrup, PhD Student Charlotte U. Jansen, Research Assistant Jesper Uhd, and colleagues have revealed a compound - 4-(2-(2-fluorophenyl)hydrazineylidene)-5-imino-4,5-dihydro-1H-pyrazol-3-amine (2) as a very potent anti-biofilm.

The result might lead to a drug able to combat the biofilm of multiresistant bacteria.

Title: *SAR study of 4-arylazo-3,5-diamino-1H-pyrazoles: identification of small molecules that induce dispersal of Pseudomonas aeruginosa biofilms*

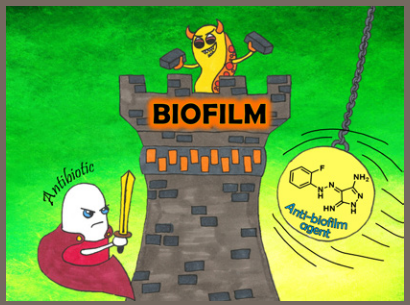


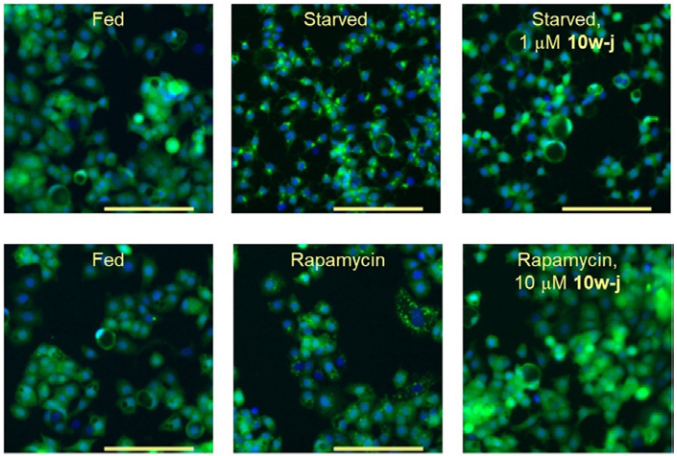
Figure: Drawing by PhD strudent Charlotte U. Jansen used as inside cover of RSC Medicinal Chemistry

Published in RSC Medicinal Chemistry
DOI:10.1039/d1md00275a

A new concept of cholesterol transport inhibitors

Associate Professor Luca Laraia, PhD Student Thomas Whitmarsch-Everiss, MSc Student Asger H. Olsen and colleagues have identified cholesterol transporting protein inhibitors and report the first potent and selective inhibitor of Aster-C within a concept that applies to other cholesterol-binding proteins.

Title: *Phenotyping Reveals Targets of a Pseudo-Natural-Product-Autophagy Inhibitor*



Published in Angewandte Chemie
DOI:10.1002/ange.202000364

New findings in the field of X-ray transient absorption

An international collaboration including Professor Sonia Coriani, Professor Klaus B. Møller, and former Postdocs Shota Tsuru and Mátyás Pápai have revealed the ^1A_u ($n\pi^*$) state of pyrazine in electronic relaxation.

Electronic relaxation in organic chromophores often proceeds via states not directly accessible by photo-excitation. The research team reports on the photoinduced dynamics of pyrazine that involves such states, excited by a 267 nm laser and probed with X-ray transient absorption spectroscopy in a table-top setup.

Their work supports the substantial role of the ^1A_u state in the photoinduced dynamics of pyrazine, as suggested by previous theoretical studies.

Title: *X-ray transient absorption reveals the ^1A_u ($n\pi^*$) state of pyrazine in electronic relaxation*

Published in Nature Communications
DOI: 10.1038/s41467-021-25045-0

A look into the structural relaxation of a polystyrene star polymer

Work by Professor Kristoffer Almdal et al. was featured as the October front cover of Physical Review Letters.

The cover photo illustrates the small-angle neutron scattering pattern of a stretched three-arm star polymer with deuterium labelling at the end of each arm.

During the steady-state flow, the scattering pattern shows two sets of independent correlations peaks, reflecting the structure of a polymer confined in a fully oriented three-armed tube. Upon cessation of flow, the relaxation constitutes three distinct regimes.

Title: *Small-Angle Neutron Scattering Study of the structural Relaxation of Elongationally Oriented, Moderately Stretched Three-Arm Star Polymers*

Published in Physical Review Letters
DOI: 10.1103/PhysRevLett.127.177801

Capturing CO_2 in solid material

With Professor Anders Riisager at the helm, researchers from DTU Chemistry are testing a new and energy-efficient method where CO_2 can be captured in solid material and upgraded to a cleaner product that can subsequently be used for producing green fuels.

The method and material are patented and being tested at a biogas plant in Sweden - in collaboration with the company Wärtsilä, which supplies sustainable technologies to the manufacturing industry.

The goal is to capture up to 90 per cent of the CO_2 from biogas with less than half the energy compared to the current common methods.

Read the full article on dtu.dk

Photo: DTU Chemistry

PhD School

PhD from DTU Chemistry

DTU Chemistry takes pride in educating PhDs at the highest international level. We offer a diverse research education in modern chemistry, which contributes to the development of cutting edge science at the department. The goal for all PhD students is to publish in leading journals and participate in leading international conferences during their three year long research education.

Power Performance

Excellent scientists must also be able to communicate their research results efficiently. Therefore, DTU Chemistry offers all PhD student an intensive communication course (1.5 ECTS) to practice their presentation techniques to perfection. A cornerstone in this regard is the annual PhD Symposium at which stakeholders from industry are invited to attend both oral presentations and a poster session by the Department's PhD students.

Contact us

On the following page, you can get acquainted with the DTU Chemistry PhD Defences of 2021. All supervisors invite you to get in touch, if you are interested in the full thesis, in further information, or in a possible collaboration.

14

Completed PhDs in 2021

23

PhDs admitted in 2021

Photo: DTU Chemistry

PhD Defences 2021

Read the summary of each project

Alexandre Voute
Bimolecular reaction dynamics and spectroscopy of weakly bound complexes
Supervisor: Niels Engholm Henriksen

Chengxin Li
Structural, biosynthetic and serological interaction studies of the capsular polysaccharides from Streptococcus pneumoniae
Supervisor: Jens Øllgaard Duus

David Nielsen
Spectroscopy and in-situ studies of environmental catalysts
Supervisor: Susanne Mossin

Huili Cao
Vanadium-based Nanomaterials for Energy Storage Applications
Supervisor: Susanne Mossin

Jie Meng
Ultrafast photophysics in Mn-doped semiconductor quantum dots for optoelectronic application
Supervisor: Kaibo Zheng

Koosha Ehtiati
Fundamental studies of polyelectrolyte brushes
Supervisor: Esben Thormann

Laura Voigt
Radical architectures in two dimensions
Supervisor: Kasper Steen Pedersen

Mingli Liang
Correlating Structure and Photophysics in Metal Halide Perovskite Crystals
Supervisor: Kaibo Zheng

Mikkel Burggraaf Buendia
First-Row Transition Metal-Catalyzed Carbon-Carbon Bond Formation
Supervisor: Søren Kegnæs

Qinying Pan
Ultrafast Excited-state Dynamics in metaled 2, 2'- Bipyridine Covalent Organic Frameworks Photocatalysts
Supervisor: Kaibo Zheng

Suk Kyu Ko
Molecular Understanding of the Effects of Stabilizing Excipients during Lyophilization of Biopharmaceuticals
Supervisor: Günther Peters

Torsha Moitra
Coupled Cluster Based Methods for Photoabsorption and Photoelectron Spectroscopy
Supervisor: Sonia Coriani

Xiaomei Yan
Electrochemical studies of redox active molecular and enzyme monolayers on nanostructured electrode surfaces
Supervisor: David Tanner

Yulong Miao
3d Transition Metal Catalyzed Dehydrogenation of Alcohols
Supervisor: Robert Madsen

World Class Education

Faculty is committed to support the education of future chemists through lectures and supervision. In addition to daily teaching, DTU Chemistry takes great responsibility for the study management of three of DTU's programmes by having three Head of Study. Professor Jens Ø. Duus is Head of Study of the MSc programme Applied Chemistry, Professor Klaus B. Møller of the BSc programme Chemistry and Technology, and Professor Mads H. Clausen of the BSc programme Life Science Engineering.

BSc admission in 2021:

143 students - **Life Science Engineering**

69 students - **Chemistry and Technology**

MSc admission in 2021:

49 students - **Applied Chemistry**

70

BEng, BSc, MSc, and PhD courses managed by faculty

Photo: Joachim Rode

Photo: DTU Chemistry

Facilities & Services

The NMR Center • DTU

is a campus infrastructure hosted by DTU Chemistry for the benefit of all departments and centers at DTU, as well as external academic and industrial partners.

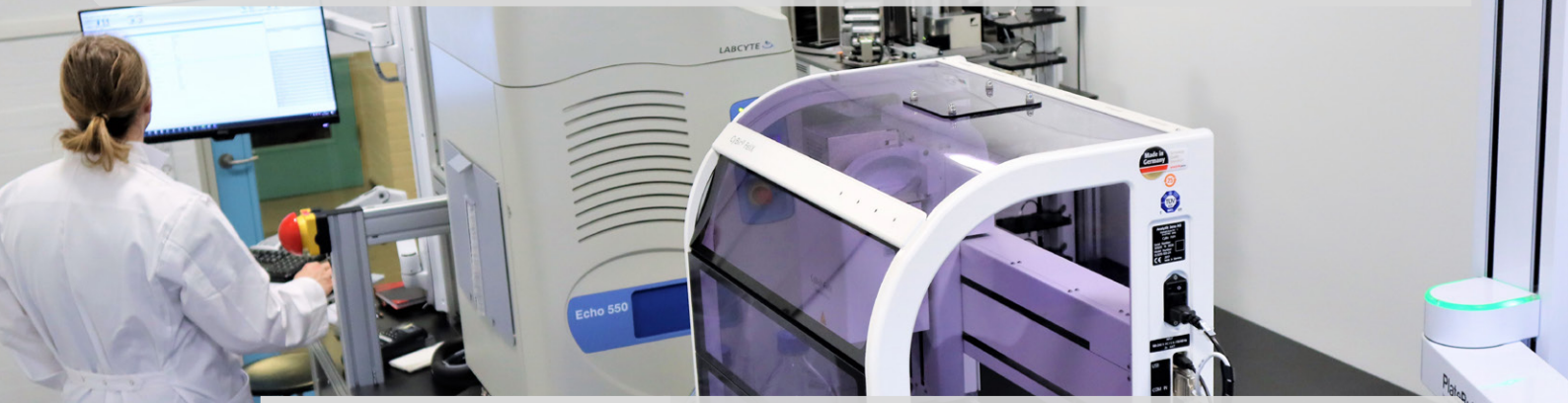
The NMR Center • DTU provides access to state-of-the-art NMR instrumentation ranging from 400 to 800 MHz.

NMR spectroscopy provides molecular information in a variety of liquid or solid samples. In doing so, NMR spectroscopy delivers an unbiased overview of molecular structures and functions. The opportunity to avoid "working blindly" vastly accelerates research projects and provides rapid quality control of chemical processes and products. Thus, NMR spectroscopy can contribute vastly to the efficient use of project resources.

For more information, please contact **nmr@dtu.dk**

DTU Screening Core (DTU SCore) is a fully automated platform for biochemical, biophysical and cell based high-throughput screening assays. The platform performs assays in 96-, 384- and 1,536-well format with multiple readout options, such as absorbance, fluorescence, luminescence, imaging etc. Thanks to close collaboration with the DK-OPENSCREEN platform, the DTU SCore facility has on-site access to a collection of 50,000 compounds.

For more information, please contact **dtuscore@dtu.dk**



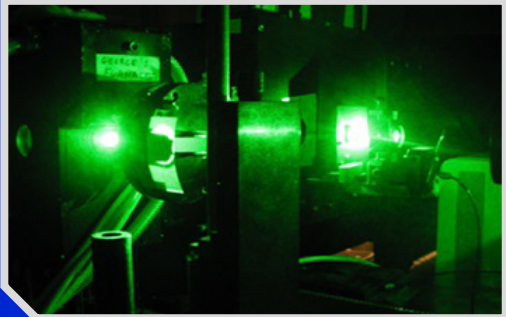
DK-OPENSCREEN is the national research infrastructure for chemical biology. In addition to the advanced compound library, located at DTU Chemistry - with room for 200,000 substances in total - DK-OPENSCREEN offers a wide range of screening facilities and highly specialized knowledge, for example on multi-resistant bacteria and phenotypic screening in cells.

For more information, please visit the website: **dk-openscreen.dk**

X-ray crystallography is a method that deals with the atomic construction of substances in solid phase such as crystals or fibers. When a crystal or fiber is irradiated with X-ray, a diffraction pattern is emitted. An analysis of this pattern provides information on the three-dimensional arrangement of atoms in the material.

We offer to solve structures for both academia and industry.

For more information, please visit the website:
kemi.dtu.dk/forskning/facilities/service-crystallography



Raman Spectroscopy is an universal analytical technique for identification of molecules in gases, liquids and solids by scattering of laser light. The Department is equipped with a confocal Raman instrument associated with a microscope and fiber optics.

For more information, please visit the website **kemi.dtu.dk/forskning/facilities/raman_spektroskopi**

Honours

Photo: DTU Chemistry

PhD receives Young Researcher Award

Former PhD student Marta Lopez Vidal received a DTU Young Researchers Award for her extraordinary accomplishments during her PhD studies. Earlier this year, Marta also received the Michael Wormit Award for her development of critically important features for treating core-level states and related spectroscopies using the highly accurate EOM-CC framework in Q-Chem.

BSc project optimizing ship engines wins Green Challenge

Signe Tronsen won the Green Challenge prize for the project *'Palladium and platinum containing zeolite catalysts for complete methane oxidation'*. Her project was performed together with Frederik Nyled Feddersen in collaboration with Umicore Denmark and aimed to remove the methane slip when using Liquified Natural Gas (LNG) as fuel. Maritime transportation is challenged by incomplete methane combustion when using some types of large LNG-fueled engines.

Photo: Mikal Schlosser

Photo: Bax Lindhardt

International award to the Head of DTU Chemistry

Erling H. Stenby, Head of Department at DTU Chemistry, was awarded the "2021 SPE Distinguished Achievement Award for Petroleum Engineering Faculty".

The prize recognizes superiority in classroom teaching, excellence in research, significant contributions to the petroleum engineering profession and/or special effectiveness in advising and guiding students.

"Some people might wonder why we need research in oil and gas in the middle of our green transition. The reason is, that this knowledge is needed to support a sustainable future – for example, we have a lot of focus on how to store CO_2 in old oil fields or other suitable geological formations. We also support the development of geothermal energy, as well as generic research within applied thermodynamics, colloid and interface science, and large scale simulations" says Erling, who has been very active in the area of CO_2 storage and capture for more than 20 years.

Outreach

Industry Project Day

In 2021, the Department hosted a hybrid Industry Project Day that took place both online and with physical attendance. Industrial partners had the opportunity to present potential projects to BSc, BEng, and MSc students from DTU Chemistry. Several companies such as Aquaporin, Novozymes, Haldor Topsoe, and Synopsys Denmark proposed interesting projects and interacted with the students. More Industry Project Days will be arranged in the future, and DTU Chemistry look forward to seeing even more companies join. For more information, please contact **fundraising@kemi.dtu.dk**.

DTU ScienceShow

DTU ScienceShow is a group of students who deliver a professional science show with entertaining and educational elements from chemistry and physics.

DTU ScienceShow is part of DTU's branding and recruiting strategies and locally hosted at DTU Chemistry with Professor Anders Riisager heading the Advisory Board.

High School Lectures

DTU Chemistry hosts a broad range of lectures such as 'Green Chemistry and Technology' for high school students.

Photo: Thomas Hjort Jensen

Student innovation

At DTU, innovation and entrepreneurship are integrated into our study programmes, mandatory courses, and electives. Through projects, events, internships, and student jobs, students gain experience within the business community, which ensures that students develop entrepreneurial competences and that, in turn, companies benefit from innovative inputs from the students.

Business collaboration

DTU has a strong tradition for working with companies and has a wide range of collaborations regarding strategic research collaborations, continuing education, student projects, conferences, etc. In 2021, DTU Chemistry had nine signed collaborative research projects with public and private companies. The interaction between the university and the business community enables theory to be put into practice and that research is based on real-world issues.

Photo: DTU Chemistry

Collaboration with industry: *Together with Novozymes, chemistry student Simone Anika Skou Olsen has been developing new methods for measuring detergent and other residues in our clothes. The research can potentially minimise skin irritation and pollution from surfactants.*

Join us

Are you interested in cooperating with DTU Chemistry?
Find the right contact person at **kemi.dtu.dk/english/aboutus/contact**

Part of a leading university - DTU rankings*

	Nordic Region**	Europe	World
Leiden Ranking Citation Impact Indicator (top 10% publications) All sciences	1	48	120
Leiden Ranking Proportion of Collaborative Publications with Industry	2	6	10
QS World University Rankings	4	35	99

* As per 27 October 2021

** The Nordic region consists of Denmark, Sweden, Norway, Finland, and Iceland

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