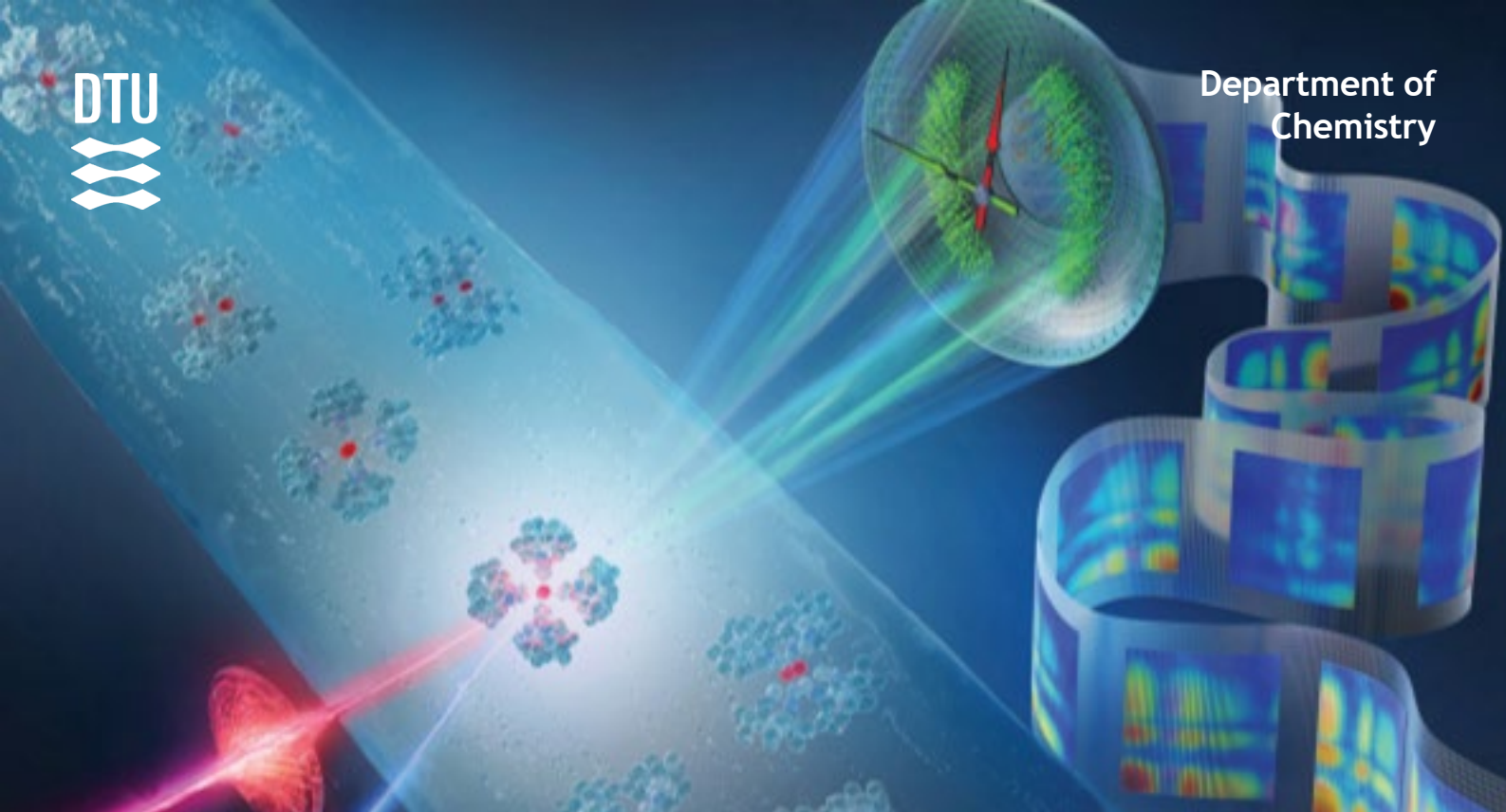




Department of  
Chemistry



# DTU Chemistry Highlights from 2023

# Contents

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Introduction	3
Research sections	4
Research in figures	5
Funding	6
Selected publications	11
Innovation	15
PhD School	16
Alliances	18
Facilities & Services	19
Honours	23
Outreach Education	24
DTU rankings	27

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# Chemistry holds the key to solving global challenges

As a central component in many solutions, chemistry is essential for establishing a sustainable future society. For instance, chemistry serves as a cornerstone for the green transition and the development of new materials. In life sciences, chemistry is used to develop vaccines for life-threatening diseases, and with quantum chemistry, we now have the opportunity to develop new methods for simulating complex chemical systems.

Chemistry is also vital in the work with carbon capture, utilization, and storage (CCUS). Thus, several researchers from DTU Chemistry are involved in the interdisciplinary green partnership INNO-CCUS.

With the development of quantum computers, quantum chemistry now holds immense potential. We are grateful to have received a new grant from the Novo Nordisk Foundation supporting a major project aimed at creating knowledge and developing methods to harness the exceptional computing power of quantum computers for quantum chemical calculations of molecular properties.

Within life sciences, chemistry is central in identifying, understanding, and treating diseases. Among other achievements, we have secured grants for developing new methods to introduce drugs into the brain, thereby advancing treatments for brain diseases.



Another project at DTU Chemistry leverages the fact that cancer cells have specific complex carbohydrates on their surface to develop vaccines for cancer treatment. Moreover, education at DTU Chemistry is an investment in the future. Every year, new skilled candidates graduate, with the majority finding employment in the industry, and we are witnessing an increasing demand for our students.

At DTU Chemistry, we look forward to a new year and to continue our commitment to offer innovative ideas and solutions for the benefit of society.

Head of Department, Erling H. Stenby

# Three major research sections

The three research sections of DTU Chemistry contribute to new knowledge and solutions in areas such as medicine, green energy technologies, and sustainable materials, benefiting both people and the environment.

## Organic Chemistry\*

The Section of Organic Chemistry is organized into three research areas:

**Chemical Biology** focuses on diverse synthesis, targeting diseases and plant biology. It aims to develop diagnostic tools and drug discovery compounds.

**Synthesis and Catalysis** focus the research on synthesizing complex molecules, creating compound libraries, and developing synthesis methods using catalysis and computer modeling.

**NMR Spectroscopy's** research involves determining structures of complex metabolites and developing new NMR pulse sequences for small, heterogeneous samples.

## Inorganic Chemistry\*

The Section Inorganic Chemistry focus on three major research areas:

**Center for Catalysis and Sustainable Chemistry (CSC)** Focus on refining biomass and waste into valuable chemicals, fuels, and materials, and on sustainable large-scale chemical production.

**Molecular Materials** engages in the design, synthesis, and characterization of nanoscale materials.

**NanoChemistry** specializes in experimental and theoretical chemical and biological nanoscale science with various applications for fuel cells and sensors.

## Physical Chemistry\*\*

The Section of Physical Chemistry focuses on the following areas:

**Theoretical chemistry** applies quantum mechanics to study molecular structure and reactivity.

**IR and THz spectroscopy** investigates weakly bound clusters using experiments and quantum modeling.

**Centre for Energy Resources Engineering (CERE)** focuses on fluid flow, hydrocarbon processing, and carbon capture and storage, with an emphasis on process modeling.

**Polymers and Functional Interfaces** engages in understanding polymer structure and designing polymers with novel properties for applications in coatings and medical technology.

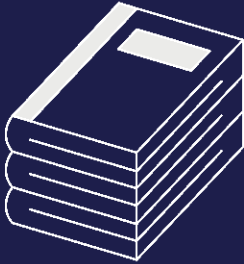
**Biophysical Chemistry** explores chemistry at the biology interface, targeting biocatalytic and biomedical uses.

\* Until 29 February 2024 these sections was a part of Section for Organic and Inorganic Chemistry.

\*\* Until 29 February 2024 this section was named Section for Physical and Biophysical Chemistry.



# Research in figures



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161

Publications in 2023  
WoS-indexed journals



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28 faculty

30 postdocs  
6 researchers and  
senior researchers



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1.24

Normalized citation impact

12.1%

Publications in top 10%



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22

BEng, BSc, and MSc projects  
completed with industry



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22

WoS publications in  
cooperation with industry



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91 MDKK

in external funding



PhD-Student Augusta Korsgaard  
Foto: Simon Koefoed Toft

## **New upcoming research area at DTU Chemistry - NUCLEAR.**

### **Professor Klaus Braagaard Møller, Supervisor**

An important part of the green transition depends on finding alternative energy sources to replace fossil fuels. Nuclear power has this year been included in the EU's taxonomy for sustainable activities.

Fourth-generation nuclear power is under development and could play a significant role in efforts to reduce CO<sub>2</sub> emissions across the international energy landscape.

Molten salt fission reactors are considered the safest fourth-generation reactors, partly due to their compact size and great design flexibility.

The goal is for fuel and fission products to dissolve in the molten salt, which would mean high utilization efficiency and secure waste management when the fission products are bound in the salt following cooling. Therefore, it is important for the development of molten salt reactors to understand and be able to quantify how fission products dissolve in a molten salt.

In collaboration with the Danish company Seaborg Technologies, which is researching into the development of molten salt reactors, this project will establish atomistic computer simulation protocols for investigating the solubility of fission products in a molten salt developed by Seaborg Technologies. The project is generously supported by the Independent Research Fund Denmark, Technology and Production Sciences, and is supervised by Professor Klaus Braagaard Møller.

With a combination of quantum mechanical and classical molecular dynamics simulations, as well as spectroscopic analysis and other experimental data, we will determine the relevant structural and thermodynamic parameters for characterizing the solubility of fission products in a molten salt.

The experimental part will be carried out in collaboration with the European Commission's Joint Research Centre.

# Funding



This year, we are delighted to announce that several of our researchers have received funding from the Independent Research Fund. The main goal of this fund is to support and promote the most original ideas and initiatives in Danish research.

To ensure that funds are allocated to the best research projects, they are awarded through an open national competition without thematic restrictions. The fund supports specific, time-limited research activities, with scientific quality being the primary evaluation criterion for fund allocation.

*Congratulations to:*

**Professor Günther HJ Peters**

*ENFACE: A Tool for Prediction of Enzyme Stability at Gas-Liquid Interfaces based on Computational Methods (2,9 mio. DKK).*

**Professor Günther HJ Peters**

*Structural basis for activation of tryptophan hydroxylase isoform 2 by phosphorylation and 14-3-3 protein binding (2,9 mio. DKK).*

**Associate Professor Kira Astakhova**

*Highly efficient chemical oligonucleotide synthesis of RNA (2,9 mio. DKK).*

**Associate Professor Jerrik Mielby**

*Origin of Selectivity in CO<sub>2</sub> hydrogenations (2,9 mio. DKK).*

**Professor Mads Hartvig Clausen**

*Selective degraders of the mitogen-activated protein kinases p38 gamma/delta (2,9 mio. DKK).*

**Professor Klaus B. Møller**

*Solvation of Fission Products in a Molten Salt Reactor (SolveMSR) (2,9 mio. DKK).*

## Søren Kegnæs received *Distinguished Innovators Grant* from NNF

Professor Søren Kegnæs has received a grant of 5.9 mio. DKK to develop novel and stable heterogeneous catalysts for converting CO<sub>2</sub> and methane from biogas into valuable syngas. Syngas is critical in the production of fuels and chemicals today and for the future energy and chemical portfolio. The project aims to achieve efficient and economic CO<sub>2</sub> utilisation which could significantly impact the environment and society.



## Martin Nielsen received 4 mio. DKK from the Villum Foundation

This recognition follows Associate Professor Martin Nielsen's upgrade from the Villum Young Investigators Programme (YIP) to YIP+.

Villum Foundation introduced YIP+, in 2021, to secure the university careers of the most talented Villum Young Investigators (YIP) at the associate professor level



## Two talented PhD students have been awarded the prestigious Fulbright scholarship

PhD students Frederik Ørsted Kjeldal and Frederik Simonsen Bro, from the groups of Associate Professor Janus Juul Eriksen and Associate Professor Luca Laraia at DTU Chemistry, have been awarded the prestigious Fulbright Scholarships.

A grant from Fulbright Denmark represents more than just financial support; it signifies a commitment to fostering academic exchange between the U.S. and Denmark. It is also a mark of distinction.

Recipients of the grant are rigorously evaluated in both countries based on their academic, professional, and personal achievements, as well as their potential to build on these accomplishments to become leaders in their fields.

## Great funding news supporting of groundbreaking research in CO<sub>2</sub> storage

The research group of Associate Professor Wei Yan have received two major grants from the **Innovation Fund Denmark** in support of their important research in CO<sub>2</sub> storage.

From the Innomission instrument **INNO-CCUS**, a grant of approximately DKK 3.9 million was awarded to the project **“Optimizing carbon capture simulation through advanced modelling tools”**.

The aim of the project is to develop accurate, robust software tools to be used in and with process simulators for variety of standard, novel and innovative carbon capture processes. Understanding error propagation is crucial for optimizing the design and operations of CCUS facilities.

Another **INNO-CCUS** grant of app. DKK 1.1 mio was awarded to the project **“Innovative Strategies to Address Salt Precipitation in CO<sub>2</sub> Storage”**, which aims to investigate salt precipitation during CO<sub>2</sub> storage operations, starting from pore-scale to field-scale.

The research seeks to enhance understanding and management of risks affecting CO<sub>2</sub> injectivity.



# Other notable funding

## Independent Research Fund Denmark

### - Independent Green Research

- Associate Professor Søren Kramer, *Visible Light-Enabled Enantioselective C-H Oxidation*, 3.2 mio. DKK.
- Professor Kasper Steen Pedersen, *Atomically Precise Metal Cluster Catalyst*, 3.2 mio. DKK.

Selected from the top proposals with a success rate of 9% in 2023, the Independent Green Research grants are awarded only to the most promising research ideas that can significantly impact the green transition.

## Horizon Europe

- Associate Professor Wei Yan, *Material Science Innovation for Accelerated, Sustainable and Safe Implementation of Carbon Capture and Storage (MISSION-CCS)*, 3 mio. DKK.
- Professor Mads H. Clausen, *GlyCanDrug*, 2.2 mio. DKK.
- Professor Mads H. Clausen, *IMPULSE*, 1 mio. DKK.

## Innovation Fund Denmark

- Partnership Director Karina M. Søgaard, *Building the INNO-CCUS Partnership*, 8.9 mio DKK

## Novo Nordisk Foundation

- Associate Professor Luca Laraia, *A targeted protein degradation strategy for the treatment of neurodegenerative disorders*, 5.0 mio. DKK
- Associate Professor Charlotte Held Godtfredsen, *Riboswitch RNA structures – important modulators of activity (RIBRNA)*, 2.9 mio. DKK

## Carlsberg Foundation

- Associate Professor Kira Astakhova, *Equipment for synthetic carbohydrate chemistry*, 0.3 mio. DKK

## Villum Foundation

- Researcher Jie Meng, *Visible-Light-Response Multiple Exciton Generation*, 2.0 mio. DKK.

# 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 2023.

For a complete list, scan the code or visit:

[kemi.dtu.dk/english/aboutus/publications](https://kemi.dtu.dk/english/aboutus/publications)

Read the



## Accurate Measurement of Diffusion Coefficients Using the CVD Method

Molecular diffusion is essential for many scientific and industrial applications, depending on accurately measured or estimated diffusion coefficients.

The constant volume diffusion (CVD) method measures liquid-phase diffusion coefficients at high pressures but needs complex analysis to interpret the data.

The results of the study, conducted by Associate Professor Wei Yan, Postdoc Yibo Yang and Professor Erling H. Stenby at DTU Chemistry, confirmed the CVD data's insensitivity to gas-phase diffusion coefficients and highlighted Michelsen's algorithm as an effective tool for processing CVD data.

The CVD method can be used within the areas of Chemical Engineering, Petro-Industry, Pharmaceuticals (drug delivery) as well as Materials and Environmental Science.

Title: *Determination of Diffusion Coefficients from Constant Volume Diffusion Tests through Numerical Simulation*

Published in Fluid Phase Equilibria  
<https://doi.org/10.1016/j.fluid.2023.113944>



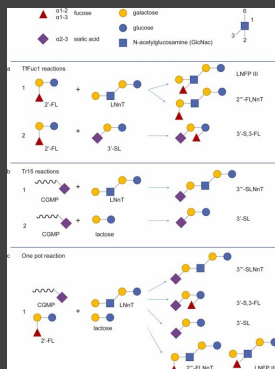
Read the full article

# Producing Human Milk Oligosaccharides (HMOs) in Cow's Milk

Human milk oligosaccharides (HMOs) are specific glycans in human breast milk, serving as prebiotics, immune modulators, and cognitive enhancers for infants. Unlike cow's milk, which lacks HMOs, producing them in cow's milk can significantly improve infant formula.

Postdoc Valentina N. Perna, Mille International ApS, has in collaboration with Associate Professor Sebastian Meier, DTU Chemistry, and Professor Anne S. Meyer, DTU Chemical Engineering, demonstrated that sialylated and fucosylated HMOs can be generated in cow's milk through enzymatic transglycosylation.

This method allows for the direct enrichment of milk and infant formulas with HMOs. Enzymatic production of HMOs can also be extended to other beverages, improving their nutritional value and health benefits for infants.



Title: *Enzymatic production of a suite of human milk oligosaccharides directly in milk*



Read the full article

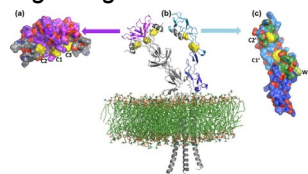
# Targeting tumor necrosis factor for treating Inflammatory and Autoimmune Diseases

The tumor necrosis factor (TNF) plays a crucial role in the immune system and is involved in diseases like rheumatoid arthritis, psoriasis, Alzheimer's, and multiple sclerosis.

TNF and its receptors, TNFR1 and TNFR2, are important targets for drug development. The review, made by international acknowledged scientists including Associate Professor Charlotte H. Gotfredsen and Professor Mads H. Clausen from DTU Chemistry, highlights recent advances in small molecules targeting TNF and its receptors and explores new strategies for modulating TNF signaling.

These developments could lead to safer and more effective treatments for inflammatory and autoimmune diseases.

Title: *Small-molecule modulators of tumor necrosis factor signaling*



Published in Drug Discovery Today

<https://doi.org/10.1016/j.drudis.2023.103575>



Read the full article

## Efficient CO<sub>2</sub> Methanation with Ruthenium Nanoparticles on Nano Magnesium Oxide

Ruthenium (Ru) nanoparticles on nano Magnesium Oxide (MgO) are very effective for CO<sub>2</sub> methanation, aiding renewable energy storage and cut greenhouse gases. The study by Postdoc Farnoosh Goodarzi, Postdoc Mikkel Kock, Associate Professor Jerrick Mielby and Professor Søren Kegnæs, DTU Chemistry, showed MgO with 5% Ru had the best performance, achieving 54% conversion at 375°C, producing 520 moles of CH<sub>4</sub> per mole of Ru per hour, and staying stable for over 50 hours. The Ru/MgO catalyst was also active at low temperatures (250°C) due to MgO's ability to chemisorb and activate CO<sub>2</sub>.

This catalyst can be used to convert CO<sub>2</sub> into methane efficiently, helping in renewable energy storage and reducing greenhouse gas emissions. It is suitable for industrial processes that aim to utilize CO<sub>2</sub> as a resource and for developing low-temperature CO<sub>2</sub> methanation technologies.

Title: *CO<sub>2</sub> methanation using metals nanoparticles supported on high surface area MgO.*



Read the full article

Published in Journal of CO<sub>2</sub> Utilization

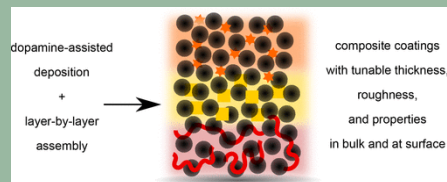
<https://doi.org/10.1016/j.jcou.2023.102396>

## Efficient Coating Preparation via Dopamine-Assisted Deposition

This study by PhD Runtian Qie, Senior Researcher Saeed Zajforoushan Moghaddam and Professor Esben Thormann explores dopamine-assisted deposition combined with layer-by-layer assembly as an efficient method for creating coatings with adjustable thickness, roughness, and functional properties.

This method leverages dopamine's versatile chemistry to co-deposit various functional materials, such as polymers, ions, and nanoparticles.

The layer-by-layer approach allows precise control over coating thickness, surface roughness, and vertical chemical composition. We demonstrated the advantages of this technique in fabricating both single- and multi-component coatings.



Title: *Dopamine-Assisted Layer-by-Layer Deposition Providing Coatings with Controlled Thickness, Roughness, and Functional Properties*



Read the full article 13

Published in ACS OMEGA

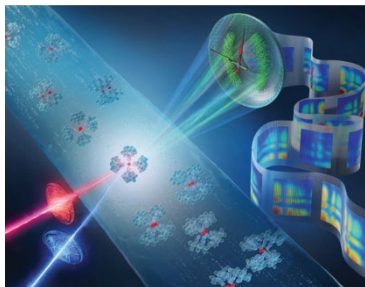
<https://doi.org/10.1021/acsomega.2c05620>

## The cover of The Journal of Physical Chemistry Chemical Physics and elected as 2023 PCCP Hot Article

An international collaboration involving more than ten academic institutions, Professor Klaus B. Møller and Associate Professor Niels E. Henriksen, DTU Chemistry, along with other prominent DTU researchers, have combined computer simulations and ultrafast x-ray experiments to investigate some of the most fundamental chemical processes.

By analyzing angular correlations in the scattered X-rays, details on the rapid dynamics, the movements and change of the molecules, can be uncovered.

The method can be applied to study fast structural dynamics of molecules in both liquid and gas phases.



Title: *Exploring fingerprints of ultrafast structural dynamics in molecular solutions with an X-ray laser*

Published in Journal of Physical Chemistry Chemical Physics  
<https://doi.org/10.1039/D3CP01257C>

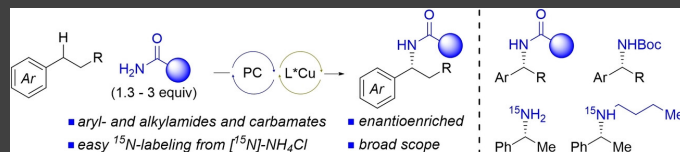


Read the full article

## New Method for Making Specialized Chemical Compounds

A new technique allows the easy creation of specific amides and benzylamines by modifying C–H bonds. This process uses minimal starting materials, along with a special copper catalyst, light, and an oxidant, working under gentle conditions. It's useful for creating a wide range of compounds, including  $^{15}\text{N}$ -labeled amides and amines starting from affordable  $^{15}\text{NH}_4\text{Cl}$  for research.

The new method, developed in a collaboration between PhD Candidate Xueming Chen, Associate Professor Søren Kramer, DTU Chemistry, and Professor Zhong Lian, Sichuan University, is efficient and versatile, making it suitable for late-stage modifications and complex chemical synthesis.



Title: "Enantioselective Intermolecular Radical Amidation and Amination of Benzylic C–H Bonds via Dual Copper and Photocatalysis"

Published in Angewandte Chemie - International Edition  
<https://doi.org/10.1002.anie.202217638>



Read the full article



# Innovation

Innovation is an important part of the work of DTU Chemistry.

In 2023, we had 32 ongoing innovative projects with commercialisation potential. The projects focus on green transition, life science, and materials science and development.

In 2023:

- 4 have received Innovation Enabling Grants for a total value of 2.8 MDKK
- 10 have reported Notifications of Invention
- 2 Software Notification Forms of software for commercial assessment

## 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 2023, DTU Chemistry had 9 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.

## Join us

Are you interested in cooperating with DTU Chemistry?  
Find the right contact person at  
[kemi.dtu.dk/english/aboutus/contact](https://kemi.dtu.dk/english/aboutus/contact)

# 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 students 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 the 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 2023. All supervisors invite you to get in touch, if you are interested in the full thesis, in further information, or in a possible collaboration.



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20

Completed PhDs in 2023

16

PhDs admitted in 2023



# PhD Defences 2023

## Frederik Hegaard

*Structural and mechanical investigations of polyelectrolyte films*

Supervisor: Esben Thormann

## Ruwei Yao

*Synthesis of an alkaloid inspired compound collection*

Supervisor: Luca Laraia

## Anna Kristina Schnack-Petersen

*On Simulating Ultra-fast Chemical Processes and their Spectroscopic Signatures*

Supervisor: Klaus Braagaard Møller

## Sofie Slott

*Precision nucleic acid diagnostics using novel oligonucleotide reagents and amplification-free assays*

Supervisor: Kira Astakhova

## Mathies Brink Sørensen

*In-Situ NMR based Metabonomics of Microbial Secondary Metabolites*

Supervisor: Charlotte Held Gotfredsen

## Nianzhe He

*Identifying oxysterol interacting proteins through specific degradation*

Supervisor: Luca Laraia

## Wenting Fang

*Selective catalytic conversion of biomass-derived furanic compounds – Design of solid catalysts and structure-performance relations*

Supervisor: Anders Riisager

## Andreas Kjær Erichsen

*Synthesis and Exploration of Large-Ring Cyclodextrins Using Enzyme-Mediated Dynamic Combinatorial Chemistry*

Supervisor: Sophie R. Beeren

## Qian Zhao

*Surface engineering and photophysics of InP/ZnS quantum dots for photocatalytic application*

Supervisor: Kaibo Zheng

## Yibo Yang

*Molecular diffusion in systems related to reservoir fluids*

Supervisor: Wei Yan

## Christina Breth Nielsen

*Nanopatterning of 2D materials by block copolymer self-assembly*

Supervisor: Kristoffer Almdal

## Josefine Hvarregaard Andersen

*Coupled Cluster-based Methods for Linear and Nonlinear Spectroscopies in Different Frequency Regions*

Supervisor: Sonia Coriani

## Nicolai Steen Broberg Hansen

*Alcohol Dehydrogenations Catalyzed by Iron(III) and Chromium(III) Catalysts*

Supervisor: Robert Madsen

## Rasmus Lykke Mortensen

*Durable catalysts for complete methane oxidation*

Supervisor: Susanne Mossin

## Alexander Tobias Nikol

*POP Pincer Complexes of Ruthenium and Manganese for Small Molecule Transformations*

Supervisor: Martin Nielsen

## Junjie Kang

*Bio-based adhesives for wet environments inspired by the natural mussel adhesive*

Supervisor: Esben Thormann

## Chantal Joseph Abou Fayssal

*Metal nanoparticles embedded in ligand-functionalized water-soluble core-shell polymers for application in aqueous biphasic hydrogenation*

Supervisor: Anders Riisager

## Deepthy Krishnan

*Mono- and bimetallic nanoparticles stabilized by functionalized ionic liquids: Synthesis and catalytic application*

Supervisor: Anders Riisager

## Kasper Hornstrup Hansen

*Templated Enzymatic Synthesis of Cyclodextrins: From Redox-Responsive Systems to Preparative Scale Synthesis*

Supervisor: Sophie R. Beeren

## Peng Wei

*Design and Evaluation of An Intranasal Carbohydrate-based Vaccine against Streptococcus pneumoniae Serotype 12F*

Supervisor: Mads Hartvig Clausen

# Alliances and strategic partnerships

As part of our ambition to extend international collaboration, we have succeeded in getting PhD Alliance Scholarships with leading technical universities in Europe.

DTU's formalized strategic alliances, the Nordic Five Tech and the EuroTech Universities Alliance, have provided DTU Chemistry with 4 PhD scholarships in 2023.

**Professor Anders Riisager and Professor Kristoffer Almdal** each has a PhD collaboration with KTH Royal Institute of Technology in Stockholm.

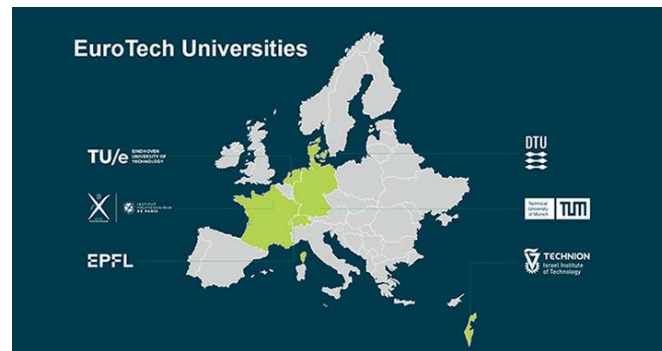
**Associate Professor Katrine Qvortrup** has a PhD collaboration with Swiss Federal Institute of Technology Lausanne.

Furthermore, **Associate Professor Kira Astakhova** collaborate with Eindhoven University of Technology on a PhD Scholarship.

The **Nordic Five Tech** is a strategic alliance of the five leading technical universities in Denmark, Finland, Norway and Sweden. The alliance was established in November 2006 with the goal of utilizing the shared and complementary strengths and creating synergies within education, research and innovation.



The **EuroTech Universities Alliance** is a strategic partnership of leading European universities of science and technology joining forces to build a strong, sustainable, sovereign, and resilient Europe.





# 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” immensely 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:

Head of the NMR Center • DTU  
Charlotte Held Gotfredsen, [nmr@dtu.dk](mailto:nmr@dtu.dk)

Laboratory Manager  
Kasper Enemark-Rasmussen, [nmr@dtu.dk](mailto:nmr@dtu.dk)



# DTU Chemistry unveils new facility for uncovering the secrets of materials with cutting-edge electron diffraction

DTU Chemistry is proud to announce the establishment of the "DTU·Electron Crystallography Facility", which was inaugurated in August 2023 and open to both academic and commercial partners.

This innovative tool allows for structure elucidation of materials for which growth of single-crystals suitable for traditional X-ray diffraction methods is impossible or impractical, and for structural studies of materials, where the quantity is limiting the use of any other techniques.



*"We are thrilled about the new possibilities that this instrument provides," said Professor Kasper S. Pedersen, DTU Chemistry. "It will greatly enhance our ability to conduct pioneering research in the multitude of fields of chemistry, materials science, and biology where structural information and structure-function relationships at the atomic and molecular level are key".*

The DTU · Electron Crystallography Facility will provide ample opportunities for fundamental insight and for revolutionizing and accelerating materials discovery of, for instance, drug candidates, heterogeneous and homogeneous catalysts, and energy materials, and will be used widely across the departments of the university and outside collaborators.

## 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-OPENSSCREEN platform, the DTU SCore facility has on-site access to a collection of 50,000 compounds.

For more information, contact Platform Manager Faranak Nami, [dtuscore@dtu.dk](mailto:dtuscore@dtu.dk)



**DK-OPENSSCREEN** 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-OPENSSCREEN 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, contact Platform Manager Faranak Nami, [fnam@kemi.dtu.dk](mailto:fnam@kemi.dtu.dk)

## X-ray Diffraction and Crystallography

provides access to the atomic-level spatial structure of crystalline materials. DTU Chemistry offers single-crystal structure determination as well as X-ray diffraction analysis of powders, thin films, fibers, etc. for both academia and industry.

For more information, visit the website: [kemi.dtu.dk/english/research/facilities](http://kemi.dtu.dk/english/research/facilities)



A photograph of a modern chemistry laboratory. The room features several white fume hoods with stainless steel tops. Large windows on the right side provide natural light and a view of the outdoors. A red sign with a white 'X' and a green sign with a white 'ON' are visible on the wall. The floor is a light-colored, polished surface. The overall atmosphere is clean and professional.

## Sustainability in Operation - in upgraded state-of-the-art laboratories for education and research

DTU Chemistry has modernized and energy-efficient laboratories, prioritizing safety, a great work environment, and a comfortable indoor climate for researchers, laboratory technicians, and students.

Key improvements include height-adjustable fume hoods, an enhanced ventilation system with local exhaust ventilation, and adjustable lighting. The laboratory design has been optimized to offer first-class functionality for both education and research.

The new fume hoods, developed through a pilot project collaboration between DTU Chemistry and DTU Campus Service, will be installed in all teaching laboratories. These fume hoods can be almost entirely turned off when not in use for teaching, as indicated by large red and green indicators in each room. As a result, electricity consumption has already decreased by 16.3% compared to the same period last year.

Additionally, the amount of chemicals used in teaching experiments, which later become waste, has been reduced by rethinking the experiment designs. This has led to a smaller CO<sub>2</sub> footprint related to transport and emphasizes safe waste disposal.

Moreover, all DTU Chemistry employees have adopted a hybrid working model, participating in online meetings whenever possible to minimize unnecessary travel.



# Honours



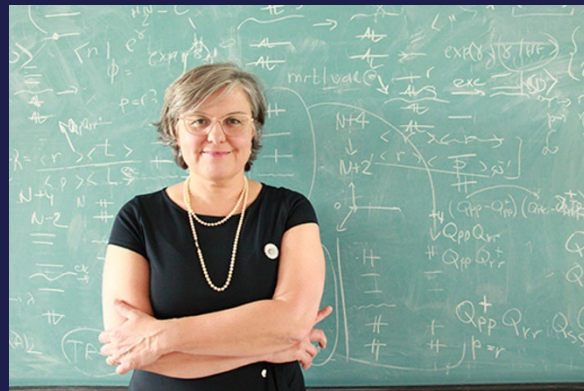
## Torkil Holm Prize - Sophie Beeren

Professor Sophie Beeren received the highly prestigious Torkil Holm Prize for her great contributions to carbohydrate supramolecular chemistry using enzymes. Dr Beeren has established a new area of research – **Enzyme-Mediated Dynamic Combinatorial Chemistry**.

The prize includes a personal grant of 50,000 DKK and is funded by the Torkil Holm Foundation.

Sonia Coriani new member of the International Academy of Quantum Molecular Science (IAQMS) and as Fellow of the Royal Society of Chemistry (FRSC)

Professor Sonia Coriani has been elected as member of the International Academy of Quantum Molecular Science (IAQMS) and admitted as Fellow of the Royal Society of Chemistry (FRSC)



# Outreach

A background photograph showing a group of young people sitting on wooden pallets outdoors. They appear to be in a casual setting, possibly a garden or a field, with trees and parked cars visible in the background. The lighting suggests it's daytime.

**Industry Project Day** In 2023, the Department hosted two Industry Project Days. 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 looks forward to seeing even more companies join. For more information, please contact **Maria Bundgaard**: [mabu@kemi.dtu.dk](mailto:mabu@kemi.dtu.dk)

**DTU ScienceShow** DTU ScienceShow consists of 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.

**Open House 2023** Open House is an opportunity for future students to learn more about our study branches and programmes, get a guided tour and listen to presentations from fully-trained engineers.

**UNF Chemistry Camp** The purpose of Ungdommens Naturvidenskabelige Forening (UNF) is to spread the interest of natural science, especially among young people. Chemistry Camp is for participants with a special interest in learning more about chemistry – practically as well as theoretically.

**Chemistry Olympiad** The Chemistry Olympiad sees talents from across the globe compete in solving both practical and theoretical challenges.





Project Day 2023

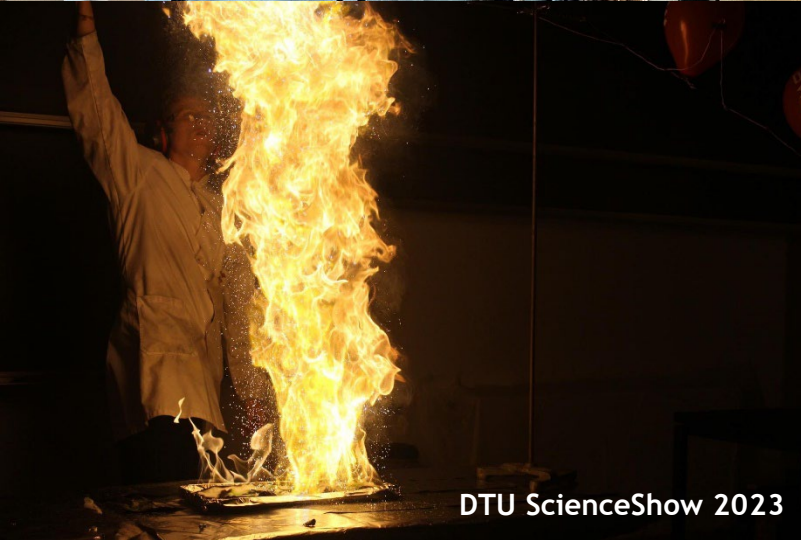


Open House 2023

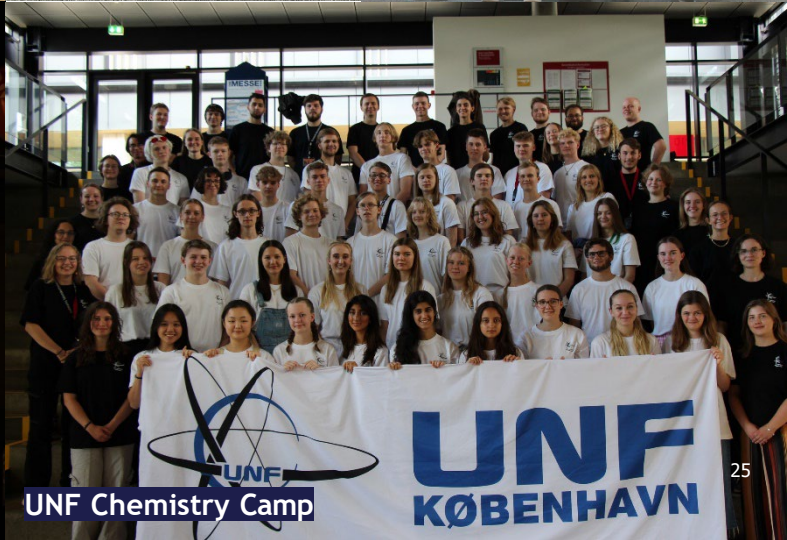


PhD Symposium 2023

Chemistry Olympiad



DTU ScienceShow 2023



UNF Chemistry Camp

UNF  
KØBENHAVN



# World Class Education

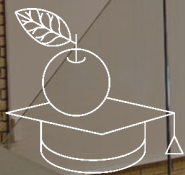
Faculty is committed to support the education of future chemists through lectures and supervision. In addition to daily teaching, DTU Chemistry takes great responsibility for the study management of three of DTU's programmes by having three Heads of Study:

- Professor Anders Riisager, MSc programme Applied Chemistry
- Professor Klaus B. Møller, BSc programme Chemistry and Technology
- Professor Mads H. Clausen, BSc programme Life Science Engineering

**BSc admission in 2023:**

**118** students - Life Science Engineering

**70** students - Chemistry and Technology



**73**

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

**MSc admission in 2023:**

**60** students - Applied Chemistry

# Part of a leading university - DTU rankings\*

## Leiden Ranking

Citation Impact Indicator (top 10% publications)  
All sciences

Nordic Region\*

1

Europe

41

World

113

## Leiden Ranking

Proportion of Collaborative Publications  
with Industry

2

5

20

## QS World University Rankings

7

51

126

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

Danmarks  
Tekniske  
Universitet

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