Department of Chemistry



DTU Chemistry

2020

Photo: Enzo Mancuso

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Flourishing research and new projects in a challenging year

The Department of Chemistry performs research, educational activities, and innovation within e.g. energy, Life Science, catalysis, and materials. Our overall aim is to contribute with new knowledge about basic scientific problems and carry out research that contributes to sustainable solutions and the achievement of the Global Goals.

Despite difficult circumstances surrounding the Covid-19 virus, 2020 has been a productive year. Our researchers have managed to maintain a high activity level and publish groundbreaking results. All courses have been executed by implementing more online classes and exams, and by applying new regulations on social distancing on campus and in the labs.

During the year, 24 PhD students graduated. The defences have been live streamed, and we are pleased to experience an increasing interest by industry and academic partners to join. It is inspiring to see how productive our PhD school is even during such challenging times. Our research groups benefit vastly from the curiosity and dedication of our PhD students.



Head of Department, Erling H. Stenby

I am excited about the future as the Department was granted 73 MDKK in external funding in 2020, which is a new departmental record. The impressive figure underlines that we have many strong research profiles and exciting new projects that address societal, environmental, and scientific challenges.

> Head of Department, Erling H. Stenby

Two major research sections

The research at DTU Chemistry is organized in two major sections. The Department takes pride in broad multidisciplinary cooperations facilitating great synergy effects across scientific areas.

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.

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

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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 behavior of small to medium-sized molecules as well as proteins, and many projects involve spectroscopy, scattering, and computer modelling.

This information is valuable for many applications, from developing effective drugs to devising new smart materials and clean energy technologies.

The research areas are biophysical and biomedicinal chemistry; IR, THz, and raman spectroscopy; high pressure phase behavior for oil and gas production; protein and x-ray crystallography; polymers and functional interfaces; theoretical, computational, and femtochemistry.

Research in figures



223 Publications in 2020 WoS-indexed journals



25 faculty 30 postdocs 10 researchers and senior researchers



1.09 Normalized citation impact 11.3% Publications in top 10%



23 BEng, BSc, and MSc projects completed with industry



39 WoS publications in cooperation with industry



73 MDKK in external funding

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 2020.

For a complete list scan the code or visit:

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



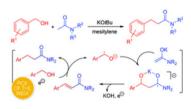


Chemical Science Pick of the Week

The journal *Chemical Science* selected the paper "Radical condensation between benzylic alcohols and acetamides to form 3-arylpropanamides" by Professor Robert Madsen and Senior Scientist Kobra Azizi as Chem Sci Pick of the Week.

The article presents an unusual radical condensation mechanism with water as the only byproduct.

The transformation is performed with potassium tert-butoxide as the only additive and gives rise to a variety of 3-arylpropanamides in good yields.



Read about their economical C-C bond forming reaction between alcohols and acetamides in *Chemical Science*.



Front cover of Green Chemistry

Associate Professor Martin Nielsen and his research group have developed a new strategy for "taming" the furanics. Their method for hydro-genating the aldehyde unit to an alcohol is so selective and effective that it has been rewarded with a Front cover in *Green Chemistry*.

Furanics include 5-hydroxymethyl furfural (HMF), 5-methyl furfural, and furfural. They are derived from (hemi)cellulosic carbohydrates and are highly promising sustainable building blocks. However, they are very prone to polymerize as well as undergoing several other undesired degradation pathways. It is therefore important to develop selective derivatization protocols for them.

Read the paper "Efficient and selective catalytichydrogenation of furanic aldehydes using well defined Ru and Ir pincer complexes" by following the QR-code.

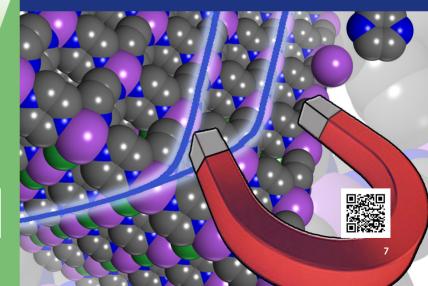


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Molecular materials as stable magnets

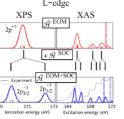
An international team – including Kasper S. Pedersen from DTU Chemistry – reports molecular materials to function as a magnet that remain stable above 200°C and resist demagnetization with 7500-oersted coercivity at room temperature. The straightforward synthetic route to the material shows promise for broad exploration of potential applications.

Metal-organic magnets with large coercivity and ordering temperatures up to 242°C Perlepe et al. *Science*, **2020**, *370*, 587



New X-ray spectroscopy method in J. Phys. Chem. Lett. L-edge

X-ray spectroscopy is one of the most powerful tools to access structure and properties of matter in different states of aggregation, as it allows to trace atomic and



molecular energy levels during various physical and chemical processes. Since theoretical modeling plays a fundamental role in revealing the information contained within the spectra, an intense effort has been directed toward developing accurate quantum chemical based methods for the treatment of core-electron spectroscopies.

A paper by Professor Sonia Coriani, PhD Marta L. Vidal from DTU Chemistry and colleagues from UCLA presents the very first equation-of-motion coupled cluster approach to compute X-ray absorption and X-ray photoemission spectra at L-edges and beyond, allowing the efficient and accurate simulation of these spectra.

The methodology has been implemented in Q-chem, one of the major comprehensive ab initio quantum chemistry software for accurate predictions of molecular structures, reactivities, and spectra.

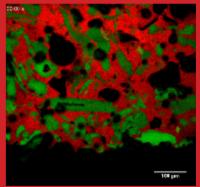


New method for water diffusion in **ACS Applied Polymer Materials**

In the work "Probing water diffusion in polymer composites using impedance spectroscopy and CARS microscopy", Professor Esben Thormann and coworkers from DTU. University of Southern Denmark, and Coloplast have demonstrated new methods for studying water diffusion in materials containing a combination of hydrophobic and hydrophilic polymers.

Water diffusion in polymer composite materials is a topic of high interest for the development for biomedical adhesives and bio-sensors.

Read more about how time-resolved impedance measurements and real-time Raman scattering microscopy provides novel

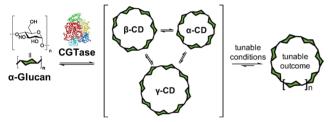


information about polymer composite structures during water uptake in the paper in ACS Applied Polymer Materials.



Proving enzyme-mediated dynamic systems to be robust and tunable

In the paper "Tuning the outcome of enzyme-mediated dynamic cyclodextrin libraries to enhance template effects", Associate Professor Sophie Bereen and Postdoc Dennis Larsen explore a system of interconverting cyclodextrins wherein the glycosidic linkage is rendered dynamic by the action of cyclodextrin glucanotransferase (CGTase).



Dynamic libraries of cyclodextrins could be obtained in wide ranges of pH, temperature, and salinity and with high organic solvent content, showing that enzyme-mediated dynamic systems can be robust and not limited to physiological conditions.

Furthermore, it is demonstrated how strategic choice of reaction conditions can enhance template effects enabling the highly selective enzymatic synthesis of specific cyclodextrins.



Cover of Physical Chemistry Chemical Physics

Protein structures derived from cryogenic electron microscopy play an increasing role in structural biology due to recent technical innovations. However, freezing may change protein structure and dynamics relative to the physiologically relevant "hot" state.

To explore this, Professor Kasper Planeta Kepp and colleagues studied the important Alzheimer protein gammasecretase by molecular dynamics as a hot, cold, and quickly cooled state in both membrane and water systems.

The paper shows that the experimental structure resembles the simulated cooled state, structurally between the hot and cold states and membrane and water systems, but with cold dynamics. "Cryocontraction" in the membrane from 303 to 85 K is observed, which reduces the size of the protein. Also, the membrane protein conformations in the membrane at normal temperature are greatly changed at low temperature and without the membrane. The study for the first time shows the importance of analyzing computationally at physiological conditions the hot-cold dynamics of cryo-structures which are becoming increasingly important in biology.

Funding



Two young researchers named Sapere Aude research leaders by Independent Research Fund Denmark

Associate Professor Kasper Steen Pedersen and Assistant Professor Søren Kramer received approx. 6.2 MDKK each through the prestigous grant from the Independent Research Fund Denmark.

Kasper Steen Pedersen: "Frustration in Molecular Tessellations"

The presence of order in the placement of atoms in a material is crucial for the properties of the material. It is therefore somewhat of a holy grail to be able to tailor materials on atomic level and thereby control how the atoms bind to each other.

Kasper Steen Pedersen will take advantage of the fact that molecular building blocks can be synthesized in different shapes and assemble themselves into new types of materials. This can lead to new possibilities for materials with applications within photonics and quantum computing.

Søren Kramer: "Asymmetric C-H Functionalization for Accelerated Medicine Synthesis"

For more than half of the approved pharmaceuticals, the active pharmaceutical ingredient can exist in two forms that are mirror images of each other containing different properties.

Søren Kramer will develop a new method that can lead to effective discovery of pure mirror images and thus accelerate the development of new drugs.





Through a joint project with Coloplast, Professor Esben Thormann has received a Grand Solution grant for OPTIMAL (Ostomy Product that is Measuring Abrupt Leakage).

In previous projects, Professor Esben Thormann, his research group, and colleagues have developed a skin simulator to test novel adhesives. The team aims to, e.g., improve the life quality of people using ostomy products.



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Rapid cancer diagnostics device funded

Associate Professor Kira Astakhova was granted 1.5 MDKK by the Innovations Fund Denmark for the spin-out project FLEET.

FLEET is a point-of-care microfluidic platform that has the purpose of tackling the lack of specificity, high cost and slow diagnosis of lung cancer with the current methods that are used. FLEET is an ultra-fast reader device able to give results in 50 minutes, while two weeks is required with the current methods for receiving diagnosis.

Projects fueled by Green Transition Grant

The Danish Independent Research Foundation granted a total of 12 MDKK to three DTU Chemistry projects that facilitate green transition within different applications:

- The project "Development of novel nanostructured catalysts" led by Professor Søren Kegnæs.
- The project "New Methods for Valorization of Glycerol" led by Professor Robert Madsen.
- The project "Deciphering and Pushing Biocatalysis in Non-Conventional Cell Factories" led by Associate Professor Sebastian Meier.

Young Researcher Fellowship will spark the development of a gamechanging method that converts CO₂ to a chemical ressource

With the project Low-Temperature CO₂ Valorisation, Associate Professor Martin Nielsen aims to develop a catalytic system that effectively transforms CO₂ to chemical building blocks that can be used industrially under very mild conditions. The project will contribute to the development of a future sustainable society. The Carlsberg Foundation granted Martin Nielsen a 5 MDKK Young Researcher Fellowship for the project.



Three original research ideas gain financial support

Independent Research Fund Denmark (DFF) has awarded more than 11 MDKK to the following four bold projects ideas at DTU Chemistry:

- The project "Predicting geochemically induced, microscopic defect escalation in geologic carbon storage across five orders of magnitude" led by Assistant Professor Yi Yang who will examine what happens when CO₂ is stored in the Danish underground.
- The project "Quantum Control of Photo-Isomeriza tion", where Associate Professor, D.Sc., Niels Engholm Henriksen aims to provide greater insight into how certain laser light can control the outcome of chemical reactions.
- The project "Computational screening tool for lipase reactions in organic media" where Professor Günther H. J. Peters will investigate how to improve enzyme activity in dehydrated media.
- The project "Chemical Engineering of Electrical Conductivity in Metal-Organic Frameworks: Towards Base Metal Electrocatalysts" by Kasper Steen Pedersen.

The Carlsberg Foundation funds new state-of-the-art research equipment

Associate Professor René Wugt Larsen received 1.2 MDKK for a THz cluster spectroscopy facility that will enable a plethora of unprecedented experimental investigations of weakly bound model systems of relevance for the energy, materials and life sciences.

Associate Professor Susanne Mossin received 0.25 MDKK for a mass spectrometer for operando spectroscopy - enabling simultaneous evaluation of both structure and activity of e.g. a catalyst in action.

Assistant Professor Luca Laraia was granted 2 MDKK for a state-of-the-art imaging system for chemical biology.

Professor Mads H. Clausen was awarded 0.73 MDKK to support the new DTU SCore infrastructure, which is currently under construction. DTU SCore is a platform for automated high-throughput screening of small molecules for biological activity, which can serve as a starting point for chemical biology research and early drug discovery.

Other notable funding

Villum Experiment

- Xinxin Xiao, "Enable bioelectro-synthesis of chiral amines (EnBioAm)", 2 MDKK
- Mads Hartvig Clausen, "A paradigm shift in carbohydrate chemistry: stereocontrolled glycosylation", 2 MDKK
- Søren Kramer, "Asymmetric Catalysis and C-H Functionalization for Sustainable Synthesis of Advanced Organic Molecules", 2 MDKK

The Novo Nordisk Foundation - NNF Project Grant Nat.Tech

- Mads Hartvig Clausen, "Formulation and immunological characterization of glycan-based cancer vaccines", 1 MDKK
- Martin Nielsen, "Sustainable synthesis of biomass-derived monomers and biodegradable polymers for biomedical applications and pharmaceuticals (BIOMED)", 3 MDKK
- Robert Madsen, "Formation of Carbon-Carbon Bonds from Alcohols by Radical Reactions", 3 MDKK

Lundbeck Experiment Grant

 Katrine Qvortrup, "Targeting nature's B-CSFB gatekeeper as a door-opener for delivery of drugs to the brain", 2 MDKK

Innovations Fund Denmark - Industrial PhD

 Susanne Mossin with Umicore, "Durable catalyst for complete methane oxidation" / Rasmus Lykke Mortensen, 0.4 MDKK



Besides the FLEET cancer dignostics device, Associate Professor Kira Astakhova is developing treatment of rheumatoid arthritis. Read the 2020 feature article about her work through the QR code.

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Photo: Bax Lindhardt

PhD School

PhD from DTU Chemistry

DTU Chemistry takes pride in educating PhDs at the highest international level. We present 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 2020. All supervisors invite you to get in touch, if you are interested in the full thesis, in further information, or in a possible collaboration.



PhD Defences 2020

Christin Alina Pohl Characterization of protein-protein interaction of single domain proteins in solution Supervisor: Pernille Harris

Daniel Hansen

Skin adhesives for ostomy care applications: Water diffusion in polymer composites & effect on adhesion Supervisor: Esben Thormann

David Benjamin Christensen Synthesis and Application of carbon materials in heterogeneous catalysis Supervisor: Søren Kegnæs

Fabrizio Monda First-Row Transition Metal-Catalyzed Dehydrogenation Reactions Supervisor: Robert Madsen Fatemeh Keshavarzi Development of substantive topicals with high sweat resistance Supervisor: Esben Thormann

Frederick Stappen Nielsen Functional gold nanomaterials and graphene platinum catalysts for electrochemical energy conversion Supervisor: Jens Øllgaard Duus

Jakob Maximilian Marinkovic Supported Ionic Liquid-Phase (SILP) Membrane Reaction Systems for Industrial Homogeneous Catalysis Supervisor: Anders Riisager

Jing Tang Development of Three-Dimensional Graphene Biocatalysts for Enzymatic Biofuel Cells Supervisor: Jens Øllgaard Duus

Read the summary of each defence



Johannes Eiler The Interplay of Viscoelasticity, Water Transport, and Adhesion in Skin Adhesives under Wet Conditions Supervisor: Esben Thormann

Junhao Huang Formation, structure, and properties of stimuli-responsive polyelectrolyte films Supervisor: Esben Thormann

Kristoffer Hauberg Møller Novel methods for synthesis of zeolites and zeolite-encapsulated metal particles Supervisor: Søren Kegnæs

Marta Lopez Vidal Development and Applications of Coupled-Cluster Methods for X-Ray Spectroscopy Supervisor: Sonia Coriani

PhD Defences 2020

Natalia Teresa Skawinska Allosteric regulation of human tryptophan hydroxylase isoform 2 (hTPH2) Supervisor: Günther H.j. Peters

Niklas Rosendal Bennedsen Design of heterogeneous metal catalysts for organic synthesis Supervisor: Søren Kegnæs

Nikolaj Sten Troelsen Synthesis and Screening of Diverse and Three-Dimensional Libraries for Fragment-Based Drug Discovery Supervisor: Mads H. Clausen

Rouzana Pulikkal Thumbayil Catalytic Conversion of Biomass-derived C1 - C3 Compounds to Value-added Chemicals Supervisor: Søren Kegnæs Simone Louise Zacho Novel Heterogeneous Catalysts with Nano-Engineered Porosity Supervisor: Søren Kegnæs

Simone Vestermann Samuelsen Metal-Catalyzed Dehydrogenation of Alcohols Supervisor: Robert Madsen

Sujata Mahapatra Protein-protein interactions in high protein concentrations Supervisor: Pernille Harris

Tao Jiang Polyelectrolyte Multilayers with Tunable Properties - Synthesis, Layer Assembly, and Post-modification Supervisor: Esben Thormann

Ulf Molich

Improving Methods for X-ray Absorption Spectroscopy Studies of Metalloproteins Supervisor: Pernille Harris

Wei Huang

Metal-organic frameworks derived nonnoble metal caalysts for proton exchange membrane fuel cells Supervisor: Kristian Mølhave

Yiqun Liu High Pressure Phase Behavior of Asymmetric Mixtures for Oil Production Supervisor: Wei Yan

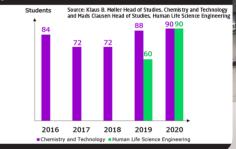
Zhiyong Zheng Extracellular Electron Transfer of S. oneidensis MR-1: Fundamentals and Applications Supervisor: Jingdong Zhang

World Class Education

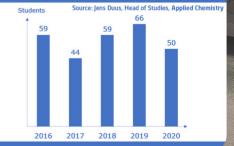
Faculty is committed to the education of future chemists and contributes to this through teaching at a high level. In addition to daily teaching, DTU Chemistry also takes great responsibility for the study management of three of DTU's programmes by having three Heads of Studies. Professor Jens Ø. Duus 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.

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BSc admission



MSc Applied Chemistry admission



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

Photo: Joachim Rode

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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.

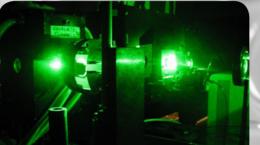
For more information, please contact **nmr@dtu.dk**



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.

The easy access to screening facilities and compound samples is aimed at increasing technological and scientific development.

Get more info or access to DK-OPENSCREEN by contacting Platform Manager Faranak Nami, **fnam@kemi.dtu.dk**



Raman Spectroscopy is an

universal analytical technique for identification of molecules in gases, liquids and solids by scattering of laser light. The Department has recently obtained a new confocal Raman instrument associated with a microscope and fiber optics.

For more information, contact Jan C. Petersen Senior Reseacher at Danish Fundamental Metrology, **jcp@dfm.dk**

Service Crystallography

DTU Chemistry performs X-ray crystallography, which 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, contact Chemist Maria Blanner Bang, **mablat@kemi.dtu.dk**



Honours

Professor Esben Thormann receives prestigious polymer award



The Danish polymer award -ATV | Elastyren Prize was given to two researchers, one of whom was Professor Esben Thormann, because; "Both candidates are internationally recognized polymer researchers who have impressive research production and have built up strong research groups within their respective research areas (..) ", the chairman of the prize committee noted.

The award includes 50,000 DKK per recipient, which is given as a personal recognition.

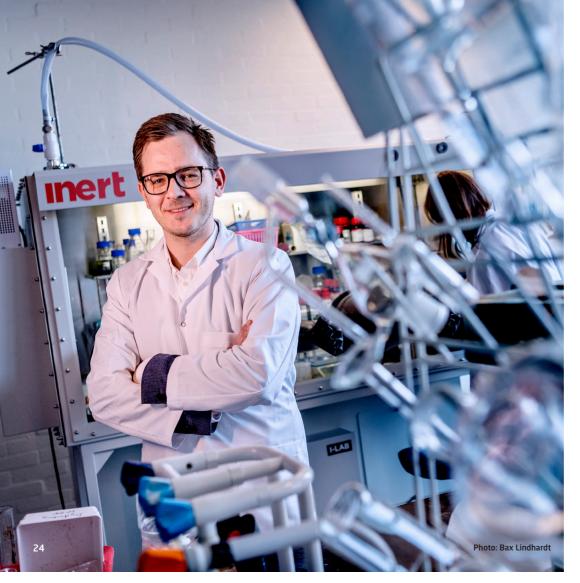


Talented PhD student receives EliteForsk travel scholarship

PhD student Mathias Thor Nielsen received an EliteForsk travel scholarship, which he will use for researching future catalysts at Harvard University in Boston.

Novo scholarship awarded MSc student

Anders Grundtvig Utzon was awarded the Novo scholarship for his thesis. He will develop a new method within asymmetric synthesis, which is used in the production of optically pure chiral substances for e.g. medicines.



Young researcher receives Kirstine Meyer´s Memorial Award

In 2020, Associate Professor Kasper Steen Pedersen was among the few researchers who were awarded the rare and very prestigious Kirstine Meyer's Memorial Award by the Society for the Dissemination of Natural Science (SNU).

He conducts research in the boundary layer between synthetic chemistry, materials science, and solid state physics.

His innovative research has already resulted in more than 50 publications in high impact journals such as *Science*, *Nature Chemistry* and *Nature Communications*.

Outreach

Industry Project Day

In 2020, 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. Due to the success of the event, more Industry Project Days will be arranged in the future, and DTU Chemistry look forward to seeing even more companies joins. Contact fundraiser Josefine Flanagan Lønholdt at **jofl@kemi.dtu.dk** for more information.

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 Spectroscopy and Identification of Organic substances for high school students.



Outreach

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 2020, DTU Chemistry had 18 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



Part of a leading university - DTU rankings*





Danmarks Tekniske Universitet

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