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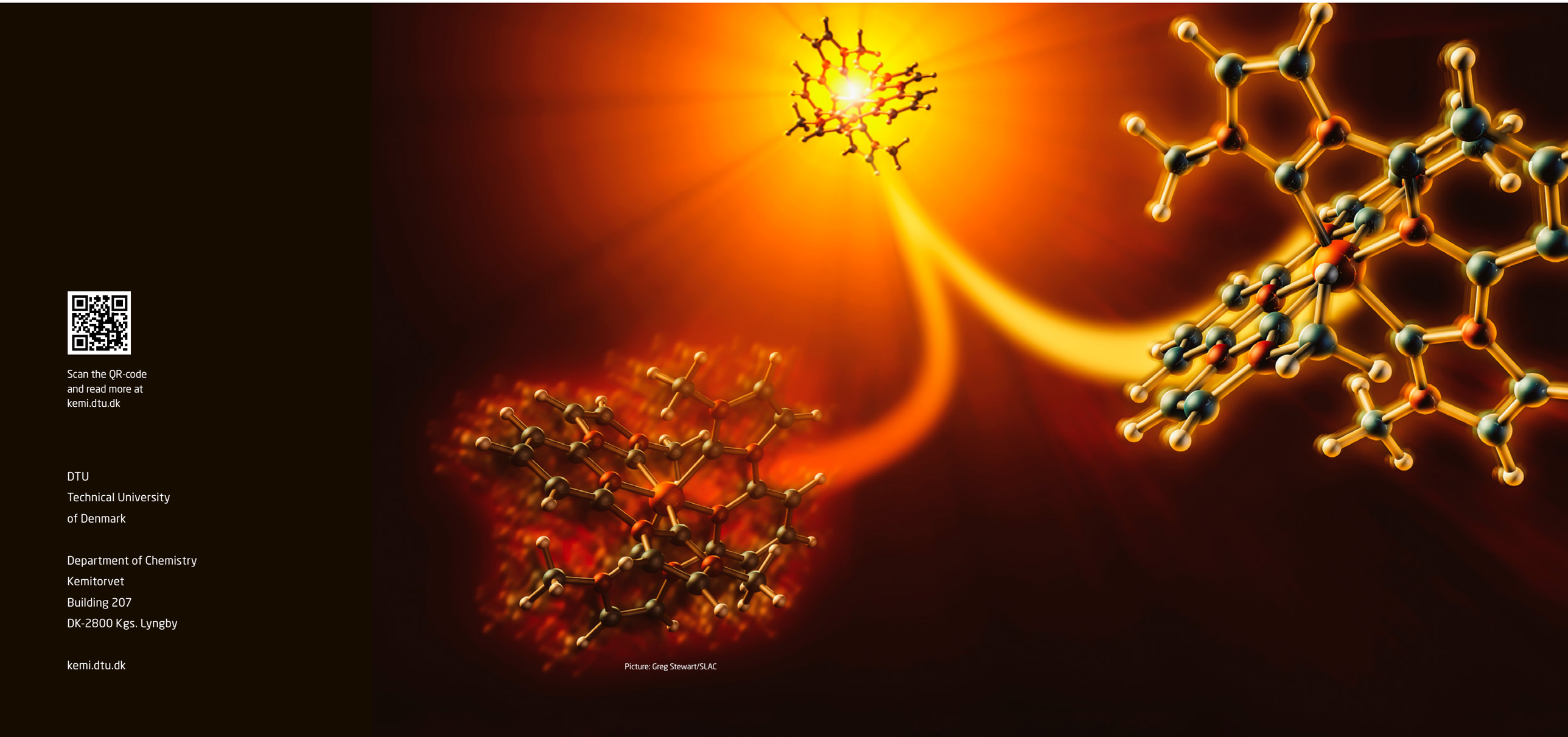
Department of Chemistry
Annual Report 2019



Picture: Greg Stewart/SLAC

A well-tuned Department

The DTU Chemistry Management Group (left to right) Lise Peitersen, Erling H. Stenby, Jens O. Duus, Inge Holkmann Olsen, and Klaus B. Møller.

Content

Welcome to the DTU Chemistry Annual Report 2019 – a year characterized by innovation, evaluation, and academic excellence.

In the fall, an international research evaluation panel consisting of four international researchers visited the Department to scrutinize our activities. The overall feedback was very positive. Especially our 'translational research' – basic research that industry and society can easily benefit from – impressed the panel. Since translational research is a core part of the 'DTU-dna', we are very pleased with the panel's focus on this area as a clear strength.

In conclusion, the panel also highlighted the successful recruitment of talented faculty in recent years as an important part of the positive path the Department is moving on. During the visit, the panel followed a well-planned schedule to get a full insight into our research – e.g. through meetings with all research areas. A poster session by the PhD students added another dimension to this insight. In the evaluation report, the panel pointed out potential areas of improvement and suggestions on how to fulfil new goals. This has inspired new ideas for the future departmental strategy.

In 2019, the researchers of DTU Chemistry were very productive. The number of Peer-Reviewed articles (228) rose by 30 % compared to 2018. Three very promising patents were obtained and currently, we have 28 ongoing patent-cases. In addition, several DTU Chemistry spin-out companies are flourishing with new investments and partnerships.

The Department takes great pride in contributing to important, groundbreaking research networks. Thus, I am excited to see several researchers at DTU Chemistry being a part of government-designated ESS Lighthouse environments. The PIPPI-consortium is currently in its final phase. Through several years, the project, well represented by members of the DTU Chemistry 'protein squad', has thoroughly investigated e.g. protein-protein interactions in relation to product formulations. The exciting work done by the consortium forms a great starting point for future protein projects.

Our researchers and advanced infrastructure are in growing demand. Researchers and companies from all over the world are reaching out to us for closer collaboration and we are glad to present some of these researchers as seminar speakers. These inspiring talks are fueling new ideas at the Department.

Significant external funding has once again strengthened our research groups with talents from Denmark and abroad. It has also made new projects possible and even new infrastructures. In 2020, the construction of the screening platform DTU SCore will begin thanks to a 10.6 MDKK grant from the Novo Nordisk Foundation. The new infrastructure at DTU Chemistry will – combined with the DK-OPENSCREEN platform – be a unique university based high-throughput screening platform in Denmark and serve as a starting point for chemical biology research and early drug discovery.

Once again, we had a record year in the uptake of new students, which shows that both 'Chemistry and Technology' and 'Human Life Science Engineering' are popular choices amongst the new generation of bright engineers. 'Chemistry and Technology' enrolled 88 students and 'Human Life Science Engineering' 60 students. Furthermore, the MSc programme, Applied Chemistry, expanded by approximately 12 % to 66 new students in 2019.

In 2019, a record number of 26 PhD students began their research at the Department while 17 graduated. It is inspiring to see how productive our PhD school is. Our research groups benefit vastly from the curiosity and dedication of our PhD students, who are closely supervised by our faculty. The PhD school assists the development of these young scientists through power performance courses, writing workshops, participation in international conferences, and close collaboration with the industry. Exclusive PhD-alliances between universities, such as EuroTech and Nordic Five Tech, are enhancing the Department's synergy and collaboration with other excellent research institutions.

All in all, 2019 has been a very productive year in all areas of the Department. We are definitely on an exciting track and doing well on projects that is part of our core dna. I hope you will enjoy this report.

Erling H. Stenby
Head of Department

Faculty: Synergy as a driving force

The research groups work effectively together across expertises, which gives a synergy effect to research at the Department. That is the conclusion from the Heads of Sections at the Department and an external evaluation panel.

"It has been an extremely productive and favourable year," says Professor Klaus B. Møller, Head of Section of Physical and Biophysical Chemistry at DTU Chemistry.

Head of Section of Organic and Inorganic Chemistry, Professor Jens Ø. Duus, continues:

“We see a faculty that has been supported for its projects by private foundations. This really strengthens the research at the department”.

In particular, the fields of biological chemistry and supramolecular chemistry have received a financial boost, but the Heads of Sections say that all research groups have positioned themselves very strongly in recent time.

In the fall of 2019, DTU Chemistry went through a comprehensive research evaluation and the department was awarded "a very high grade" by an external evaluation panel of high-profile scientists. The panel praised the individual strengths of each research group and great synergy effects across the Department, including the PhD school, as well as technology transfer efforts.

The two Heads of sections also highlight that faculty, in 2019, have been very productive in regards to publications – in fact, a record number – and several of these were published in high-impact journals.

Two new faculty members

In connection with the reallocation of faculty from DTU Nanotech, DTU Chemistry received two strong researchers.

Associate Professor Mogens Havsteen Jakobsen joined Organic and Inorganic Chemistry. He has worked with the development of innovative sensor technologies in environmental, biomedical, and security applications. Along with him, he brings the invention CRIM-TRACK – a digital sniffer dog that can detect various chemical substances. According to Head of Section Jens Ø. Duus, Mogens has brought strong analytical skills.

The section of Physical and Biophysical Chemistry now has Professor Kristoffer Almdal in the fold. He is interested in polymers as a class of materials. From a fundamental perspective, he is strong on subjects such as the development of polymer synthesis methods, the physics of polymer melts and solutions, and especially self-organization phenomena. From a more applied aspect, he does research on functional polymeric nanoparticles and sensors, polymeric biomaterials, polymer degradation, adhesion, and interfaces in polymer composites.

“Kristoffer is a huge capacity in the field of polymers and materials. With him and e.g. Professor Esben Thormann we are somewhat of a powerhouse in the field of research, and it has positioned us very well when it comes to both basic research and research aimed at the industry,” says Professor Klaus B. Møller.

Takes pride in teaching

All of Faculty is committed to the education of future chemists and contributes to this through teaching at a high level. A good example is Professor Robert Madsen who won the award as ‘Lecturer of the year’ at DTU (read more under Highlights pp. 32).

As a new initiative DTU introduced evening teaching in 2019 and DTU Chemistry was in the front line with implementation and successful execution of evening teaching in a core course in physical chemistry, commended by the Dean.

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 Human Life Science Engineering.

▲ ***Physical and Biophysical Chemistry**: Günther H. J. Peters, Wei Yan, Irene Shim, Niels Engholm Henriksen, René Wugt Larsen, Klaus B. Møller, Esben Thormann, Kasper Planeta Kepp, Sonia Coriani, Kristoffer Almdal, Pernille Harris, and Kenny Ståhl.*

Sections

Organic and Inorganic Chemistry

The Section of Organic and Inorganic Chemistry comprises 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; bioelectrochemistry; graphene nanoparticles; coordination chemistry; chemical biology; NMR spectroscopy.

Physical and Biophysical Chemistry

The Section of Physical and Biophysical Chemistry 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. The research areas are Biophysical and Biomedicinal Chemistry; IR, THz, and Raman Spectroscopy; High Pressure Phase Behaviour for Oil and Gas Production; Protein and X-ray Crystallography; Polymers and Functional Interfaces; Theoretical, Computational, and Femtochemistry.

Two new Professors continue protein research

In 2019, long-time faculty members Pernille Harris and Günther H. J. Peters were appointed Professors at DTU Chemistry. They will continue research into the properties of proteins, which is an important field when it comes to developing sustainable solutions for protein-based pharmaceuticals and industrial enzymes. Recently, both Pernille and Günther have been working on a major pan-European Horizon 2020 project called PIPPI. The aim of the project - which is in its final phase - is to map the excipients that can make proteins stable, resulting in a database containing raw data with information on the effects of the excipients and interactions with proteins. In their day-to-day work, Pernille and Günther work closely together in an iterative process. Where Pernille mainly studies proteins by using of X-ray scattering, light scattering, and other spectroscopic methods, Günther performs calculations and modeling on the computer.

▶ ***Organic and Inorganic Chemistry**: Jens Ø. Duus, David Tanner, Susanne Mossin, Robert Madsen, Charlotte Held Gotfredsen, Søren Kegnæs, Anders Riisager, Rasmus Fehrmann, Jingdong Zhang, Mads H. Clausen, Mogens Havsteen Jakobsen, Kasper Steen Pedersen, Sophie Beeren, Katrine Qvortrup, Luca Laraia, Kira Astakhova, and Martin Nielsen.*

Recruiting enzymes for new tasks in chemistry

By combining enzymology with supramolecular chemistry, the group of Sophie Beeren is paving the way for more sustainable production of chemicals.

Enzymes are the biological equivalent of catalysts in chemical industry: they speed up reactions between other compounds without being consumed in the process. But what if enzymes could perform the same job in the industry? Associate Professor Sophie Beeren heads efforts at DTU Chemistry in enzyme-based synthesis.

"Organic chemistry can achieve amazing things, but does have shortcomings in relation to sustainability," says Sophie Beeren.

Typically, chemical synthesis of complex molecules requires multiple steps, each followed by a purification process, and typically producing various biproducts. This leads to high costs, energy consumption, and generation of waste.

"If we can replace some of the traditional chemical synthesis in industrial production with enzyme-mediated processes, we can develop more sustainable processes. This is because enzymatic processes are fast, specific, and take place under mild conditions," says Sophie Beeren.

Molecular templates amplify synthesis

The real novelty in the work of Sophie Beeren is the overall concept, a non-traditional approach to the use of enzymes, which she calls Enzyme-Mediated Dynamic Combinatorial Chemistry:

"Normally, an enzyme-catalysed reaction will be like a one-way street. Starting with given reactants, the result will be a single product. The process is kinetically controlled. Instead, we propose to employ enzymes that catalyse reversible reactions between molecular building blocks to generate dynamic mixtures of interconverting oligomeric products. To achieve selective synthesis of specific products, we will exploit artificial molecular templates that bind to, stabilize, and thus amplify the synthesis of products that we chose. We exploit Nature's catalyst – enzymes – to do chemistry for us, because they are incredibly efficient. But we try to convince them to generate different products in the lab, to those they would normally make in biological systems."

Despite the many reasons to prefer enzyme-mediated production over traditional chemical synthesis, a general transition could obviously not happen all at once. The strongest case for the new paradigm can be made for relatively complex molecules. This is because the more complex the compound, the more steps it will take to produce it by traditional synthesis – and the larger the cost will be in terms of money, energy, and waste generation. Oligosaccharides are particularly challenging targets.

Biocompatible molecules for drug delivery

The group is currently looking at Large-Ring Cyclodextrins (LRCDs). These are unusual nanoscale macrocyclic oligomers of glucose that are promising as biocompatible and biodegradable hosts for stabilization, delivery and release of functional bioactive molecules. The "guest molecules" could be drugs, diagnostic markers, flavours or aromas.

Graphic textbook illustrations will show cyclodextrins as nice, rigid truncated cone-shaped molecules, each with an internal cavity able to contain a guest molecule. And indeed, this is true for the smallest and commonly available cyclodextrins α, β and γ, formed from 6, 7, and 8 glucose monomers each.

"Large-ring cyclodextrins, however, are flexible and little explored. We want to elucidate their actual structures, and also establish which guests can bind inside them," says Sophie Beeren.

In the case of LRCDs, there is a clear connection between size and functionality. As the molecule becomes larger, it becomes more flexible, opening up the possibility to host and transport larger guest molecules.

"Actually, quite large LRCDs are generated in the enzymatic production of the common smaller cyclodextrins, but within minutes will they degrade into smaller ones, because they form reversibly and the smaller cyclodextrins are more stable. Therefore, production of the larger LRCDs has previously been regarded as impractical. We have preliminary results showing that it is indeed possible to stabilize the larger LRCDs by the use of molecular templates. So far we have been able to stabilise the formation of LRCDs with up to 10 glucose units." says Sophie Beeren.

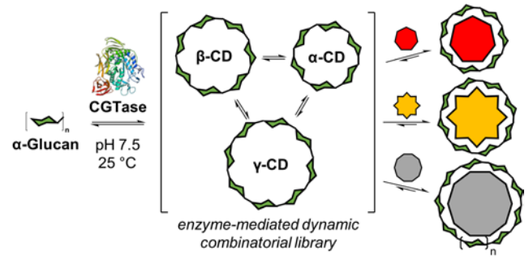
Possible applications in food and pharma

Initially, the group showed that the enzyme cyclodextrin glycosyltransferase (CGTase) can be used in the presence of artificial molecular templates to selectively synthesise the three common small CDs from α-glucan under thermodynamic control. Further, synthetic molecular templates are utilised to favour larger LRCDs, which have nine and ten glucose units respectively.

"If we can stabilize, isolate and study LRCDs in the 15-17 monomer range, I would be more than happy," says Sophie Beeren.

While enzyme-mediated production of LRCDs could find applications in the food, pharmaceutical, and cosmetics industries, Sophie Beeren emphasizes that her research is fundamental:

"Our role is not to develop or optimise processes for implementation in industry but rather to explore new ideas, and provide novel and creative approaches. Still, we do find the LRCDs especially interesting, because they are extremely difficult to access using traditional approaches. Here, we see an area where we will not just suggest a way towards more sustainable production, but also develop new and hopefully useful materials."



Cyclodextrin glucanotransferase is used to generate a dynamic mixture of cyclodextrins starting from various glucans. Addition of suitable templates induces a change in cyclodextrin distribution.

The Beeren Group

Sophie Beeren is Australian. She moved to the United Kingdom in 2006 to undertake a PhD at the University of Cambridge. In 2011, she accepted a position as Postdoc at the Carlsberg Laboratory in Copenhagen and went on to become Researcher at DTU Chemistry in 2015, then Assistant Professor in 2017 and Associate Professor in 2019.

In the near future, the group will increase substantially in size due to new grants. At the time of writing, the group consists of Sophie Beeren, three PhD Students and one Postdoc. Over the coming years, two additional PhD students and three Postdoctoral researchers will be hired. Sophie Beeren is one of just 28 researchers to receive a Carlsberg Foundation Young Researcher Fellowship grant amounting to 4.5 MDKK. The Novo Nordisk Foundation has also realised the potential and groundbreaking nature of Sophie Beeren's research and have awarded a 2.87 MDKK under the funding instrument Biotechnology-based Synthesis and Production Research.

Sophie Beeren has published a long range of scientific articles in the Journal of the American Chemical Society (JACS), Angewandte Chemie, and other prestigious journals.

Associate Professor Sophie Beeren
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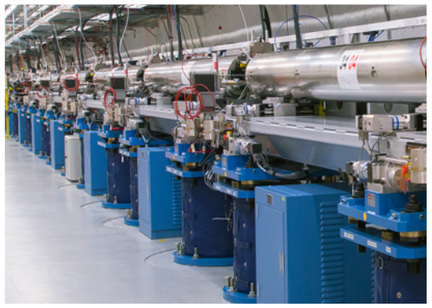
Professor Klaus B. Møller and colleagues had precious beam time at the European XFEL facility in May 2019.



The Linac Coherent Light Source (LCLS) at Stanford University.

A peek into the molecular engine room

By combining X-ray scattering at Stanford University and computer simulations, DTU researchers are able to study how molecules re-distribute energy internally.

When disturbed, a chemical system will immediately strive to find a new equilibrium. This is common knowledge in chemistry, but by just which mechanisms will the adjustment happen? An ambitious international project led by researchers at DTU Chemistry and DTU Physics has opened the door to the study of processes happening internally in molecules.

As an example, internal molecular energy distribution is of interest to solar cells. Improving photovoltaic material efficiency – measured by how large a proportion of the solar energy received will be converted into electric power – is an ongoing effort. And this is far from the only possible application, notes Klaus B. Møller:

"Very often does the occurrence of a chemical reaction depend on a localized, elevated level of energy. So, if we are able to understand how and when energy will concentrate in a given area inside a molecule, we may be able to create the right conditions for that to take place. This will potentially speed up reactions significantly – and this could in principle apply to a multitude of different reactions."

Fierce competition for beam time

The processes of interest occur at the femtosecond scale (a femtosecond is 10^{-15} second). Also, they occur at the nano-scale, meaning that many quantum mechanical phenomena are involved. In other words, measurements are extremely challenging.

"Ironically, the smaller an object you want to study, the larger an instrument will you be in need of," Klaus B. Møller smiles.

In this context, the large instrument is the The Linac Coherent Light Source (LCLS) at Stanford University, USA. The core of LCLS is a kilometre-long X-ray free-electron laser (XFEL). The laser is able to generate ultra-short X-ray pulses that hit the sample and elucidate the behaviour of individual molecules in a sample.

Using the exact right wavelength, an optical laser is able to create a sub-population of molecules by excitation. The excitation makes these molecules stand out, which facilitates studying them.

Obtaining beam time at the LCLS is an achievement in itself. Globally, only some four-five facilities at this level exist, and competition for beam time is fierce.

Simulations and experiments interact

The newest facility is the European XFEL in Hamburg, which opened in 2017, and where Klaus B. Møller and colleagues had beam time in May 2019.

"Each time, we need to do extensive computer simulations in order to establish that what we have in mind is actually possible. And later, as we get the beam time and experiments are initiated, we will do several simulations interacting with experiments. It is characteristic of this field that you can never rely on experiments alone. Without simulations, you cannot be sure that what you observe is actually what you think you observe," Klaus B. Møller comments, underlining that the opposite is also true:

"We cannot rely on simulations alone either. We need experiments to back them up. This is an ongoing interplay."

The experiments at LCLS are set up by the group of Senior Researcher Kristoffer Haldrup and Professor Martin M. Nielsen, DTU Physics, while the computer simulations are mainly done in the group of Klaus B. Møller at DTU Chemistry. Often numerous scientists from several countries will be involved. For instance, more than 40 researchers from a handful of countries are credited in recently accepted papers in the prestigious journals Angewandte Chemie and Nature Communications.

"Coordinating a project like this is actually a task in its own right. Not only does the project involve a lot of people, but they also come from different disciplines and different scientific cultures. Sometimes, one has to devote more effort to securing that everybody is onboard and happy, than to doing science! That is maybe not to everybody's liking, but personally I enjoy this side of the work. No group in one country would be able to do this kind of work alone." Klaus B. Møller says.

New area: Looking at ground-state molecules

Recently, a smaller strongly DTU-based research team – including also Associate Professor Niels E. Henriksen from DTU Chemistry – has begun exploring a new type of investigations. Instead of preparing samples for excitation studies, they do almost the opposite. Here, the laser beam wavelength is designed to counteract the normal vibration of the molecules. In other words, the molecules in this sub-population stop vibrating.

The magnitude of this achievement is illustrated by the fact, that an article based on the project has been published in the top scientific journal Physical Review Letters.

"We are able to extract these "frozen" molecules from our further considerations. What interests us is not this sub-population, but instead what happens to all the other molecules. How will these ground-state molecules react to the disturbance that we induced?"

To illustrate, Klaus B. Møller uses a metaphor:

"Suppose you are looking at a lot of people moving around in a busy central city area. Everybody is walking in different directions but since there are people everywhere all the time, it is difficult to make observations about how people will move around in a city. If you, however, remove all people in for instance one square, you can learn a lot from seeing how this void will be filled again. This is what we do in the experiment. We see how the ground-state molecules react to the disturbance – in other words, how the system regains its equilibrium."

Surprising role of the solvent

The initial "freezing" of a sub-population of molecules is done with ultraviolet light. The subsequent study of the ground-state molecules is done by stroboscopic X-ray shattering.

Asked about unexpected results from the experiments, Klaus B. Møller replies:

"We were surprised by the role of the solvent. Intuitively, you would assume the presence of a solvent to facilitate the fast return to equilibrium, as the solvent introduces more degrees of freedom to the system. However, we saw that the solvent can actually have an adverse effect by blocking internal channels used by the molecule to redistribute energy."

The molecule studied in the experiments is "PtPOP", a model system for photo-catalysis studies. One advantage is the relative harmony of this molecule. By selecting a molecule that would not snap back into the original equilibrium too fast, the researchers gained the time needed to study the various interim processes.

"We are not yet at a stage where we can just study any molecule we would like to," Klaus B. Møller admits. "However, as we will hopefully increase our skills in this discipline further, we expect to broaden the types of molecular systems we can look at. Ground-state studies open a new playing ground. After all, nearly all chemical reactions happen when molecules are in their ground-state."

Professor Klaus B. Møller
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A novel approach to treatment of Rheumatoid Arthritis

Sprung from DTU Chemistry, start-up company IBIO TECH has patented a prodrug which could become the first product that not just dampen Rheumatoid Arthritis symptoms, but actually cures patients.

Rheumatoid Arthritis (RA) is an autoimmune disease and chronic inflammatory disorder associated with progressive disability and reduced life time expectancy. Affecting around 1 % of the world's population, RA has large socio-economic costs.

RA is characterized by synovial inflammation and tissue damage. The origin and cause are unknown, and no cure currently exists. However, treatments that reduce the symptoms and the activity of the disease have emerged over the last three decades. The standard of care treatment is by disease-modifying anti-rheumatic drugs (DMARDs), where methotrexate (MTX) is the frontline drug.

Now, Danish start-up company IBIO TECH has patented a prodrug based upon an entirely new concept.

"Our drug candidate is designed to reach the synovial fluid and bind key antibodies at the site of inflammation. This will provide both a more effective treatment and a much lower level of side-effects compared to other drugs that are not equally specific," explains IBIO TECH founder Kira Astakhova, Associate Professor at DTU Chemistry.

Positive effect in the most severe cases

The targeted antibodies are ACPA (anti-cyclic citrullinated peptide antibody). A large group of RA patients has elevated levels of ACPA – they are said to be sero-positive. ACPA is both indicative of the RA diagnosis and a target for medicinal treatment. As the IBIO TECH prodrug – for the time being still referred to under its "lab name" ANC0031802 – binds to ACPA, the level of the antibodies decreases, leading to milder symptoms and eventually stopping progress of the disease.

It should be noted, that the prodrug is not universal for RA patients. Some patients do not have elevated levels of ACPA, and 15-20 % even have lower-than-normal levels, i.e. they are sero-negative. ANC0031802 will only help sero-positive patients.

"Around 60 % of RA patients will benefit from the treatment. Still, these are both the most severely affected by the disease and the hardest to treat," Kira Astakhova comments.

First clinical trials in 1.5 years

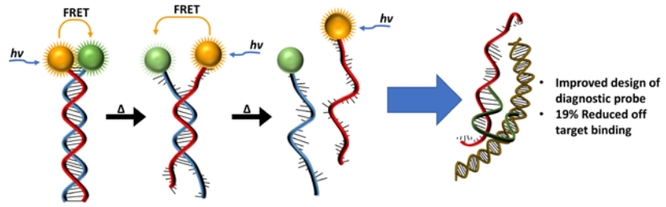
For patients in acute need of a RA cure today, the young company is unfortunately not able to assist. For obvious reasons, pharmaceutical development is subject to strict regulation and high safety standards. Therefore, it takes a long time from a drug candidate is discovered until it can enter the market. About ten years is the normal time frame. IBIO TECH has completed the first two years of this journey.

About 18 months from now, ANC0031802 should become ready for phase 1 of clinical trials. If the clinical results are satisfactory, the product will proceed to phases 2 and 3, involving a large number of patients in several countries, before, eventually, the final drug approval can be applied for.

Somewhere along that timeline, costs will rise to levels beyond the capacity of any start-up company.

"At that point we will have to exit the development, meaning we will sell or license the product to an existing pharmaceutical company with the economic capacity necessary to take the product through the final stages and into marketing," says Kira Astakhova, estimating this exit to take place about six years from now:

"That is, if we do not encounter any unpleasant surprises like unforeseen side-effects."



Associate Professor Kira Astakhova researches within synthetic biology – an interdisciplinary area between chemistry and biology that aims to design and redesign of biological components and systems.

However, even in a worst-case scenario where IBIO TECH would have to abandon ANC0031802, it would not have to be the end of the story:

"Our real invention is actually not the product itself, but a technology platform capable of delivering several similar products. So, should ANC0031802 fail for some unforeseen reason, we will able to come up with alternative candidates very quickly. In fact, we are already working on some other prodrugs as backups. But obviously, we would have to reconsider our milestones, and patients would have to wait longer before they can be offered the treatment."

Endemic to Scandinavia

While ANC0031802 can only benefit the 60 % sero-positive RA patients, the patients with normal ACPA levels and the sero-negative patients are far from forgotten, Kira Astakhova emphasizes:

"Our goal is not just to develop medicine. We also strive to understand the underlying mechanisms. From a scientific point of view, it is really interesting how the disease manifests itself so differently in different people. We know that a large genetic component exists. If we can disclose the more specific genes involved, we will be able to be even more specific as to which patients will benefit from which drugs."

Another mystery is how RA is endemic to Scandinavia. While 8 % of the Scandinavian population is at risk of developing RA, the number is less than 1 % on a global scale.

"This is an astonishingly high number," Kira Astakhova comments. "This underlines the relevance of founding a company with RA as its focus here. We do not need to look far to get the clinical samples we want. And again, it seems that genetic factors are a part of the explanation."

A better understanding of the genetics involved should also help the diagnostic abilities, Kira Astakhova hopes:
"It is a major problem, that patients are often diagnosed at a very late stage where the prognosis is much worse than if treatment was commenced earlier on."

Why late treatment is risky

After RA onset, the level of ACPA is typically very high and increasing rapidly. Here, it is absolutely necessary to reduce the level of ACPA, as otherwise the patient will be severely handicapped and may possibly die. In effect, the only method to achieve this reduction within an acceptable timeframe is by inhibiting the signalling protein TNF (tumour necrosis factor). Inhibiting TNF has a significant downside, since – as suggested by the term tumour necrosis - the protein plays a key role in the body's anti-cancer defence by identifying cancer cells and trigger their death.

"So, while most patients with RA in an advanced stage will have their symptoms reduced through TNF inhibition, this comes at the price of an increased risk of cancer. Therefore, it is highly desirable that RA is diagnosed in the early stages where it is still possible to control ACPA levels in less drastic ways than by inhibiting TNF," explains Kira Astakhova.

"Early diagnosis will benefit all RA patients, including the ones that we hope will be able to benefit from treatment with our drug candidate."

Associate Professor Kira Astakhova
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IBIO TECH

Founded in 2018, IBIO TECH today has a staff of five: CEO and Business Developer Daniel Zalomajev, CTO Sangita Khatri, Clinical Developer Tue Wenzel Kragstrup, Founder Kira Astakhova, Associate Professor at DTU Chemistry, and Co-Founder Professor Mads H. Clausen, DTU Chemistry.

The company is based on ongoing fundamental research by Kira Astakhova in the field of nucleic acid and peptide aptamers. Her interests include ultra-specific nucleic acid binding and nucleic acid/peptide/anti-body interactions. The research is supported by development of thermodynamic and optical detection techniques with applications in strategies for nucleic acid and peptide synthesis.

Kira Astakhova has received several prestigious grants including the Sapere Aude Elite scholarship, the NIH (National Institutes of Health, USA) grant, and Villum Young Investigator Grant.

Smart chemistry to save vast amounts of CO_2

Aldehydes are manufactured in large quantities by chemical companies all over the globe. A new process co-developed at DTU Chemistry will reduce carbon emissions from aldehyde production by as much as 80 %.

Detergents, fragrances and flavourings are examples of products made in large quantities with aldehydes as starting point. Given the scale of aldehyde production, a new energy efficient process co-developed by researchers at the Centre for Catalysis and Sustainable Chemistry at DTU Chemistry is about to make a significant contribution to climate change mitigation.

More than 10 million tons of aldehydes are manufactured each year. Aldehydes are produced from alkenes which are unsaturated hydrocarbons that contain carbon-carbon double bonds. Normally the alkenes are obtained as by-products from fossil feedstock in the petrochemical industry. However, they may also be produced from renewable feedstock like biomass.

"While research many places – also at DTU Chemistry – strive to produce alkenes from biomass, this is not the focus of the present project. What we have developed is a new technology able to convert alkenes into aldehydes in a far more energy efficient and environmentally benign way compared with traditional production. The key idea is to integrate two processes – reaction and separation - which are normally performed as consecutive steps into just one step in a combined reactor system, thereby minimizing energy use for the total production," says Professor Anders Riisager, DTU Chemistry.

Combing two processes in one

Alkenes are converted into aldehydes by a reaction type known as hydroformylation. Here, a formyl group (CHO) and a hydrogen atom are added to the carbon-carbon double bond in the alkene forming either a linear or a branched aldehyde. Various versions of the process exist, but they all involve high pressure of syngas, CO and H_2 (in the 10-100 bar range), elevated temperature (80-200 °C) and the presence of a transition metal catalyst. Usually the process is designed to produce mainly the linear aldehyde.

Hydroformylation of alkenes has been around since 1938, and regardless of the variety of specific setups, the basic chemistry has remained the same – and will continue to be so, also when the new process become implemented. The main change in comparison to the traditional use of hydroformylation is the new focus on creating more energy efficient processes – both in order to save energy costs and contribute to climate change mitigation.

Unlike most other chemical industry processes that produce bulk chemicals in huge quantities, the hydroformylation of alkenes is carried out by homogeneous catalysis. Instead of directing a continuous flow of liquid or gas phase feedstock through a solid, porous catalyst (this is the usual form of heterogeneous catalysis), the catalyst and the feedstock are dissolved in a liquid solvent and the catalyst only recaptured later.

"Homogeneous catalysis is generally avoided for large-scale industrial applications due to the need for recapture of the catalyst. However, in this case homogeneous catalysis is necessary in order to obtain the desired selectivity towards the linear aldehyde molecules and because the aldehydes have an unfortunate tendency to react mutually into larger molecules. If a heterogeneous catalyst was used, these molecules would accumulate in the solid, porous matrix gradually deactivating the catalyst. By adding the catalyst directly into the feedstock solution this problem is avoided," explains Anders Riisager, noting that hydroformylation of alkenes is the largest existing application of homogeneous catalysis.

Avoiding vaporization

The new process is developed by Danish company LiqTech International, German company Evonik Performance Materials together with academic groups from CSIC Madrid, RWTH Aachen, University of Erlangen-Nuremberg and DTU Chemistry. A rhodium-based catalytic complex catalyses the hydroformylation. While this in itself is not extraordinary, the real development is the integration of the catalysis and the product separation in one process using an ionic liquid system immobilized in a porous ceramic monolith with an outer polymeric membrane installed in the reactor. An ionic liquid is defined as "a substance composed of two distinct ions that is liquid below 100°C".

In other words, an ionic liquid has a very high boiling point. This is essential because the amounts lost due to vaporization are close to zero when operated in a continuous gas phase system even under elevated temperature. The ionic liquid is integrated into a so-called SILP – Supported Ionic Liquid Phase – catalyst. SILP systems are a long-standing research area at DTU Chemistry. The concept allows for high efficiency due to a highly exposed surface of the ionic liquid phase resulting in excellent diffusion dynamics. Further, the SILPs can be designed as highly selective for the given purpose – in this case immobilization of the rhodium-based catalytic complex.

"The overall solution allows for continuous operation of the catalyst in the reactor with simultaneous removal of products. Any potential problem with loss of catalyst or deactivation of the catalyst is prevented, and importantly we are able to perform the process with just 20 % of the energy use in the industry today," says Anders Riisager.

The ceramic monolith is manufactured by LiqTech in Ballerup, which specializes in silicon carbide materials for applications mainly in the water sector. Evonik Performance Materials will head the overall implementation of the technology.

High level of technical readiness

The partners have developed the new process in a joint project with EU financing, ROMEO. Following the successful initial development, the partners have been granted a further project, MACBETH.

"The fundamental technology has been proven, and we are now ready to move from research and closer to industrial implementation. To use the EU terminology, the MACBETH project will take the technology to technical readiness level 7, meaning demonstration in an industrial operational environment," says Anders Riisager.

The MACBETH project began November 2019 and will run for 4.5 years.

The new process is optimized for production of pentanal from C4 raffinates with butenes, but is viable for gas phase production of other aldehydes from other types of alkenes.

"We have demonstrated the system to be especially effective for production of pentanal from butenes. Satisfyingly, we are able to obtain very close to 100 % selectivity to pentanal and operate for several thousand hours without catalyst deactivation."

Pentanal is mainly used as the starting point for production of plasticizers, flavourings, in resin chemistry, and for rubber accelerators.

Professor Anders Riisager
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Schematic drawing and photograph of the cylindrical porous monolith consisting of a SiC core, SiC skin, and silica wash-coat. Detailed schematic drawing of the pore structure before and after liquid impregnation.

Shedding Light on Molecular Recognition Mechanisms

New experimental approaches are unveiling the weak non-covalent forces between molecules that historically have been challenging to study in the arduous terahertz spectral region.

Molecular recognition, the mechanisms by which biological macromolecules interact either with each other or with other various small substrates with high specificity and affinity to form specific molecular complexes, constitutes the foundation for all processes in living organisms. Proteins, the most important class of biological macromolecules, all realize their vital biological specific functions through the association to other molecules.

Knowledge of the detailed mechanisms responsible for molecular recognition phenomena and an accurate quantification of the energetics, which drive the association processes, will therefore help to facilitate the discovery, design, and development of new drugs.

"The *intra*-molecular vibrational 'fingerprints' of stable molecules, kept together by covalent chemical bonds, are usually detected in the infrared (IR) spectral region. However, as the non-covalent intermolecular forces stabilizing weakly bound molecular complexes normally are 10-100 times weaker than covalent bonds (~5-50 kJ·mol^{-1}), the *inter*-molecular vibrational modes introduced by the complexation between molecules are detected in the less accessible terahertz (THz) spectral region", says Associate Professor René Wugt Larsen, who is in charge of the THz cluster spectroscopy group at DTU Chemistry.

The accurate interaction strength, directionality and cooperativity of the weak "contacts" associated with non-covalent intermolecular forces can be probed *directly* via these large-amplitude modes arising from the now hindered rotational and translational motion of the subunits relative to each other. These resulting THz spectral signatures are thus crucial in order to characterize with unprecedented accuracy the intermolecular potential energy surface spanned by the subunits and yield rigorous experimental benchmarks to validate or improve quantum chemical methodologies.

However, the relevant part of the spectrum is denoted the "THz gap" as historically it has been challenging to produce intense radiation with these wavelengths. The only high-brightness sources of broadband THz radiation are offered by large-scale synchrotron radiation facilities as Canadian Light Source, Synchrotron SOLEIL (Paris), Australian Synchrotron and recently at the free-electron laser facility FELIX (Nijmegen).

"There is a fundamental need for experimental approaches which are able to investigate the intermolecular energy balances associated with the interplay of weak non-covalent forces such as directional intermolecular hydrogen bonds and dipole-dipole interactions, non-directional long-range van der Waals forces and steric repulsion between molecules", says René Wugt Larsen.

Soft "Quantum Crystals"

The demand for THz spectral signatures of weakly bound molecular van der Waals complexes has urged for the development of complementary experimental approaches employing conventional radiation sources, where the experimental sensitivity is governed by significant number densities of transient molecular systems trapped in ultra-cold inert environments.

The research group of Associate Professor René Wugt Larsen has recently demonstrated that highly enriched *para*-H_2 "quantum crystals" of >99,95 % purity offers multiple advantages as a host for low-temperature THz cluster spectroscopy arising from the unique "quantum nature".

The H_2 molecule exists as two spin isomers: *para*-H_2 with paired nuclear spins or *ortho*-H_2 with unpaired nuclear spins, where the latter has a "reactive" magnetic moment. In the ground state of this soft material, the *para*-H_2 molecules provide an almost field-free host medium, where the large-amplitude zero-point lattice motion offers significantly free space for embedded guest molecules and the crystal behaves as an "extremely cold gas".

In newly developed experimental setups the research group of Associate Professor René Wugt Larsen has been able to characterize in great detail the large-amplitude vibrational motion of weakly bound molecular van der Waals complexes embedded in enriched *para*-H_2 at 4 K.

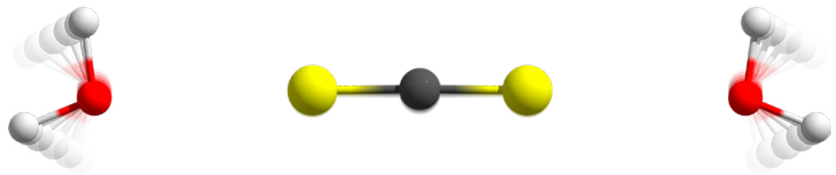
Proof-of-Concept at DTU Chemistry

The project was initiated in 2013, when René Wugt Larsen obtained a 5-year Sapere Aude Research Leader grant from the Independent Research Fund Denmark / Natural Sciences (FNU). Later, the Danish Hydrocarbon Research and Technology Centre (DHRTC) has provided further funding. The "proof-of-concept" has recently been published in the journal *Physical Chemistry Chemical Physics*.

"In this work, we have revealed interesting molecular recognition processes and we have managed to trap a variety of exotic molecular systems. These molecular systems are formed due to the kinetics associated with the mobility of molecules in the soft *para*-H_2 medium and would never form under ambient conditions", says Associate Professor René Wugt Larsen. "The observed THz signatures and intermolecular force fields provide challenging experimental benchmarks even for the most sophisticated quantum chemical methodologies", he continues.

The PhD Students Dmytro Mihrin and Alexandre Voute have developed a fully-automated cryogen-free *para*-H_2 synthesis apparatus based on a temperature controlled closed-cycle helium cryo-cooler for these studies and the workshop at DTU Chemistry has constructed many vital parts for these new experimental facilities.

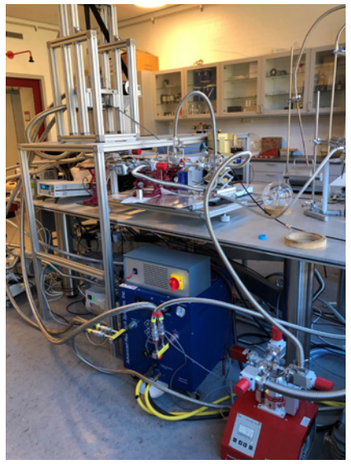
A future aim is to address one of the most fascinating phenomena in nature referred to as the "homochirality of life". The chemistry of life is built almost exclusively on left-handed amino acids and right-handed sugar molecules. Often one chiral form of a drug is active, while the other(s) are either inactive or have severe adverse effects. It has been argued, that a true breakthrough in our understanding of these molecular chirality recognition phenomena can be achieved by accurate THz spectroscopic investigations of chiral drug-receptor model systems.



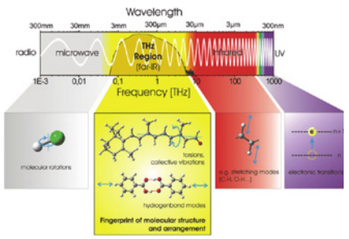
The large-amplitude hindered internal rotational motion for a kinetically formed "exotic" conformation of the ternary CS_2-$(H_2O)_2$ van der Waals complex in para-H_2.

Other Research Activities

The THz cluster spectroscopy group of Associate Professor René Wugt Larsen has recently established fruitful internal collaborations with the DTU Chemistry molecular material research groups of Associate Professor Kasper S. Pedersen and Associate Professor Martin Nielsen concerned with the spectroscopic characterization of novel metal-organic frameworks and organometallic complexes. In addition, a close external collaboration with the Danish Hydrocarbon Research & Technology Centre (DHRTC) has recently been established related to spectroscopic investigations of fluid-fluid and surface-fluid association mechanisms.



The new THz cluster spectroscopy experiment for investigations of weakly bound molecular van der Waals complexes doped in para-H_2 "quantum crystals" at 4 K.



The electromagnetic spectrum and the variety of spectroscopies (MW, THz, IR and UV) associated with the different quantum states of molecular systems [adapted from Anal. Bioanal. Chem. 2010, 397, 1009-1017].

Associate Professor René Wugt Larsen
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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.

PhD ChemClub

The PhD students at DTU Chemistry are strengthening their professional and social network at the Department. They do this through the PhD ChemClub. PhD students run the ChemClub, and they arrange several annual events: PhD Symposium, post-graduate career events with experts from industry and academia, inspiring talks by invited speakers, and social gatherings. We invite interested candidates to have a look at our website kemi.dtu.dk/English, where you can read more about our PhD programme as well as the DTU Chemistry research areas.

Power Performance

Excellent scientists must also be able to communicate their research results efficiently. Therefore, DTU Chemistry offers each 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 the industry are invited to attend both oral presentations and a poster session by the Department's PhD students.

Contact us!

In the following pages, you can get acquainted with the DTU Chemistry PhD Defences of 2019. All supervisors invite you to get in touch, if you are interested in the full thesis, in further information, or in a possible collaboration. You are also welcome to contact the Head of the PhD School, Professor Erling H. Stenby, Head of Department, ehst@kemi.dtu.dk

The 2019 edition of the PhD Symposium - held at Konventum, Elsinore - was filled with interesting presentations and posters. Several industry partners showed up and got a first hand impression of the PhD school at DTU Chemistry. They were impressed by the overall level of research and presentation techniques.

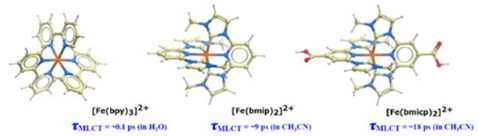
Atomistic Mechanisms of Functional Molecules

The global demand for energy is rising and for a long time solar energy has been considered as one of the best renewable and clean alternatives to unsustainable energy sources. One of the big challenges in using solar energy is to make its conversion and storage cheap, which is of particular importance in large-scale production of solar cells. This requires finding low-cost, earth-abundant, and environmentally friendly materials. In this regard, theoretical chemistry methods by providing a deeper knowledge and understanding play an important role as a complementary tool alongside experimental techniques and in development of new and high efficient materials.

This PhD thesis targets theoretical investigations on transition metal complexes and photoswitchable organic molecules, two classes of materials relevant for solar energy conversion and storage, using a wide range of theoretical approaches. The main results of this project are atomistic insights into the mechanisms behind a variety of light energy conversion processes.

A deep understanding of the photorelaxation processes occurring upon light absorption would be necessary for designing and developing more efficient materials. Quantum description of the photorelaxation dynamics in the presence of solvent is not feasible due to an exponential growth of computational time with the increase of nuclear degrees of freedom. On the other hand, it has been evidenced that the solvent can alter the dynamics of the solute molecule significantly.

The thesis provides a reliable scheme for describing solvent structural dynamics using MD simulations and shows that implicit the polarizable continuum model (PCM) can provide a trade-off between accuracy and computational cost for accounting for the solvent effects on the solute intramolecular relaxation processes. This opens for the possibility of using these solvation approaches in quantum dynamics simulations of photorelaxation processes.



The molecular structures of Fe(II) polypyridine deriv-atives and their MLCT lifetimes in H_2O and CH_3CN solutions.

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2/3 Independent Research Fund Denmark, 1/3 DTU Chemistry

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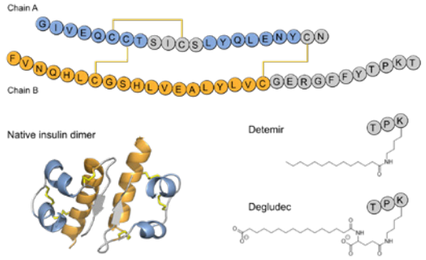
Protein structure and protein-protein interactions in formulation

The use of biopharmaceuticals in the treatment of diseases such as diabetes, cancer, and hemophilia has increased dramatically over the past decades. Despite their many advantages such as high potency, specificity, and low toxicity, many biopharmaceuticals suffer from inherent chemical and physical instabilities and short plasma half-lives, which make their formulation development and delivery challenging.

Lipidation is a successful strategy for extending the half-lives of peptide drugs through lipidation-induced self-association and association to albumin. Though albumin-association is exploited by several approved lipidated peptide drugs, structural knowledge about the albumin-peptide complexes and their interactions on the atomic level is limited. This thesis treat self-association and albumin-association of two lipidated insulin analogues, insulin detemir and insulin degludec, through an interdisciplinary approach using small angle X-ray scattering (SAXS) and molecular dynamics (MD) simulations.

The first solution structures of a detemir trihexamer, and albumin–insulin analogue complexes in 1:6, 1:12, and 2:12 stoichiometries based on SAXS data were modeled, and equilibria for albumin-detemir and albumin-degludec mixtures were proposed. The albumin-detemir hexamer solution structure shows four possible detemir binding sites. These binding sites were investigated by MD simulations and molecular mechanics Poisson-Boltzmann surface area free energy calculations. The overlapping FA3-FA4 binding site on albumin was found to be the most favorable detemir binding site.

The presence of albumin was found to enhance detemir's stability against freeze-thaw and agitation stresses almost independently on complex formation, suggesting that albumin-detemir complex formation does not lead to further stabilization.



Schematic representations of the sequences of native insulin, degludec and detemir.

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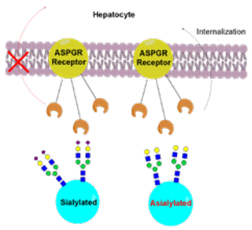
Development of detection-receptors for sialic acids

Sialic acids are a diverse family of carbohydrates widely distributed in human tissues and specifically present in both N- and O-linked glycans, where they constitute the terminal residue of the oligosaccharides on glycoproteins. Sialylation is important to a protein´s function and its physical and pharmacokinetic properties, and the ability to monitor the degree of sialylation is important in the development of protein-based drugs.

Novo Nordisk produces a drug based on a glycoprotein called Recombinant Activated Factor VII (rFVIIa), better known as Novo-Seven®, taken by patients with haemophilia or other coagulation deficiencies. In adults, the pharmacokinetics of rFVIIa is directly dependent on the number of attached sialic acids. rFVIIa is isolated as a mixture of compounds with different degrees of sialylation and no further purification is performed. The aim of this project was the development of small organic molecules able to selectively recognize sialic acid and suitable to be incorporated into a chromatographic purification system.

The first methodology explored was dynamic combinatorial chemistry. Dynamic combinatorial libraries of potential receptors were generated using reversible disulfide bonds to connect building blocks under thermodynamic control. When the target is added, the distribution of the species in the library changes leading to an amplification of effective receptors. The amplified receptors were isolated and the binding studied both qualitatively and quantitatively using 1H-NMR spectroscopy and a UV spectroscopy indicator displacement assay.

The second approach was combinatorial chemistry. Synthetic methodology was developed for the high-throughput solid phase synthesis of cyclic peptides. Three cyclic peptides libraries were synthesized. Among the three different high-throughput methods of analysis that were tested, a competitive direct ELISA assay was selected as the most suitable and reliable. The three libraries were analyzed and four potential receptors were found.



Mechanism of action of ASPG receptor. Asialoglyco-protein receptors in the liver are able to recognize only non sialylated serum protein. Thus, sialylated protein are protected from uptake and degradation.

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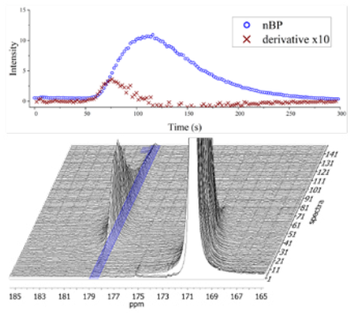
Chemical reactions and intermediates followed by DNP NMR

Modern analytical chemistry has sought to develop "in-situ" methods of analysis. These methods examine the system while the reaction is happening, allowing the characterizing of catalysts in their working state, and the observation of chemical transformations in real time.

This thesis has developed the application of dissolution dynamic nuclear polarization (dDNP) nuclear magnetic resonance (NMR) spectroscopy. This technique adds an extra, preliminary step to conventional NMR, increasing the otherwise low sensitivity of the method ten-thousand fold.



Activation study of [Rh(NBD)(DPPB)]ClO₄: nBA

NMR is one of the most common methods for discovering the structure of organic molecules. By enhancing the method using dDNP, we facilitate a number of otherwise unfeasible in-situ investigations.

Prior work using dDNP has primarily investigated metabolic and medical systems. In this thesis, we seek to expand the scope of the method by demonstrating its applicability to catalytic systems. The systems investigated were the formation of solketal, a green additive to diesel; the hydrogenation of olefins, a commonly used chemical reaction; and the 2nd generation Hoveyda-Grubbs catalyst, used for metathesis reactions.

The application of the method to catalytic systems was successful, providing a number of interesting results. It was demonstrated how we could follow the reactions of catalytic systems in real-time, observing the consumption of substrates and formation of reaction intermediates and products. Changing the conditions during the reaction, by reducing the hydrogen flow, had a direct, observable impact. The method was also utilized for analyzing the structure of a catalyst, and the changes incurred to the structure as the catalyst was activated or inhibited.

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2/3 Danish National Research Foundation, 1/3 DTU Chemistry

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Cobalt-Catalyzed Dehydrogenation of Alcohols and Amines

Usually, reactions with hydrogen gas are catalyzed by the platinum metal group, and there is therefore a great interest in finding cheaper alternatives. Cobalt is one of the commonly available transition metals, and cobalt compounds also possess interesting properties that are relevant in catalytic reactions.

The thesis describes two projects, both of which deal with hydrogen gas evolution with in situ cobalt catalysts. In the first project, a homogeneous cobalt catalyst has been formed in situ from cobalt (II) bromide, zinc metal, and a special phosphine ligand. The compound thus formed catalyzes the coupling between alcohols and amines to form the corresponding imines by the liberation of hydrogen gas and water. The mechanism has been investigated with a number of labeled substrates and the catalytically active compound is believed to be a cobalt (I) complex with the particular phosphine ligand. This complex reacts with the alcohol and cleaves off two hydrogen atoms in the same step, releasing the aldehyde and subsequently forming the imine. Hydrogen gas is then liberated from the catalyst and the catalytically active compound is restored.

Multiple reactions submitted to the same temperature were run on Radleys carousel connected to the Schlenk line, in order to perform efficiently the largest number of tests under the same conditions.

In the second project, dicobalt octacarbonyl has been heated, thereby decomposing into cobalt nanoparticles. These particles catalyze the coupling between two amines by releasing hydrogen gas and ammonia, thereby again forming imines as the product. The coupling can take place both between two different amines and as a self-coupling of a single amine. The nanoparticles have been characterized microscopically and they were found to have a narrow distribution with an average diameter of 2 nm. The heterogeneous cobalt catalyst can be isolated from the amine coupling and reused in a new reaction. In summary, in this project an in situ-formed cobalt catalyst was developed from the cobalt carbonyl complex and trioctylphosphine oxide, for the acceptorless dehydrogenation of amines into imines.

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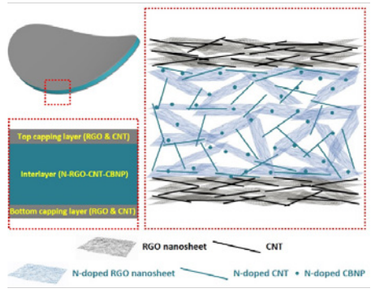
Development of detection-receptors for sialic acids

Wearable biomedical electronic devices (WBEDs) can be attached to human epidermal tissues and used for analyzing diverse health-related chemical/biological signals. Wearable sensors and power devices, which are mainly constituted by flexible composite electrodes (FCEs), are generally regarded as two functional core components of WBEDs. Therefore, developing advanced FCEs capable of realizing high-performance physiological index monitoring, energy storage or even both of them has attracted considerable research attention.

In recent years, due to their multiple function and performance superiorities, carbon-based paper-like films have been preliminarily exploited as advanced substrates of FCEs.

This Ph.D. project is devoted to the design, fabrication, characterization and application of novel carbon-based FCEs. Employing a series of facile, efficient, and scalable fabrication techniques, the engineering of three types of carbon-based paper-like films are explored. The films include nitrogen-doped hybrid dimensional nanocarbon based paper electrodes, gold nanoparticles decorated reduced graphene oxide papers, and copper cobaltate nanowires loaded on activated graphite papers.

Then these carbon-based paper-like films are either directly used as high-performance FSSSC electrodes, or employed as advanced flexible substrates to load different electrode active materials and realize superior bifunctional features. Based on a series of structural and compositional optimization, the carbon-based FCEs developed in this Ph.D. study possess excellent comprehensive performances towards energy storage or/and biosensing. Moreover, compared with other types of FCEs, the carbon-based FCEs developed in this Ph.D. study exhibit prominent practical advantages, such as low cost and facile fabrication.



Schematic illustration of the N-RGO-CNT-CBNP-P structure.

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China Scholarship Council

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Qijin Chi

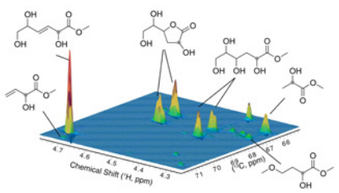
NMR Spectroscopic Exploration of Tin-Catalysed Biomass Conversion

In the pursuit to replace fossil resources with more sustainable alternatives, the chemocatalytic conversion of carbohydrates provides an important method for producing new functional chemicals. This PhD project focuses on the use of a Sn-Beta zeolite catalyst for the conversion of glucose, xylose and glycolaldehyde in methanol, to form α-hydroxy esters, such as methyl lactate and methyl vinyl glycolate (MVG), with interesting potential as building blocks for polymer production.

The project is concerned with the development and use of NMR spectroscopic methods to identify and quantify several new products in the catalytic reaction without having to purify samples or isolate new substances. Among other things, two new interesting molecules were identified from the carbohydrate conversion, namely methyl 2,5-dihydroxy-3-pentenoate (DPM) and methyl 2,4,5-trihydroxy-3-pentanoate (THM). The yields were optimized by varying several reaction conditions, yielding 19.4 % of THM and 42 % of DPM. It was subsequently shown that DPM could be used to prepare polymers.

Alkali salts such as potassium are known to modify the reaction selectivity of the Sn-Beta catalyzed carbohydrate conversion so that the transformation follows a different reaction pathway and primarily yields methyl lactate. This influence was investigated further, leading to three findings: 1; the effect was proportional to the ratio of alkali salt and tin atoms in the catalyst, 2; the reaction selectivity is under kinetic control, and 3; alkali salts facilitate breaking of carbon-carbon bonds. The reaction mechanistic pathways were investigated using carbohydrates with isotope-labeled hydrogen and carbon atoms. The key findings from this were that isomerization competes with dehydration to determine the selectivity for DPM / THM. In addition, it indicates that all carbohydrates remain connected to the tin in the catalyst until fully reacted.

Overall, this project has contributed many additional details about the Sn-Beta catalyzed conversion of carbohydrates through the study of intermediates, product distributions and the tracking of atoms during the reactions.



^{1}H-^{13}C spectral region of secondary alcohol CH-groups (indicated by small spheres) adjacent to carboxylic groups, showing the signals of both known and new α-hydroxy esters formed from conversion of glucose.

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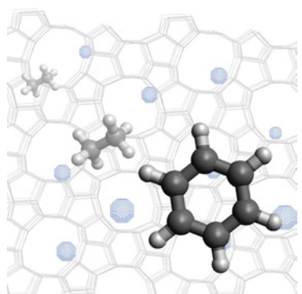
Peter Fristrup

Designing zeolite-based catalysts for production of fuels and chemicals

The world is struggling with different challenges such as depletion of fossil fuels, growing gap between energy demand and production, and most importantly emergent environmental issues. Therefore, alternative environmentally friendly resources for production of chemicals and energy are necessities. However, the transition and utilization of new resources requires development of novel technologies.

Thus, the aim of this thesis was to develop new efficient catalysts and investigate their performances in different energy and chemical production processes such as CO_2 hydrogenation to methane, methanol-to-hydrocarbons, and dehydroaromatization of ethane. In particular, MFI structured zeolites with 3-dimensional channels including ZSM-5 and silicalite-1 were employed in the presented works. Different morphologies of MFI zeolites were synthesized, characterized and applied in catalyst design. More specifically, zeolites were used as catalyst support for metals and/or as solid acid catalysts in solid phase for aforementioned chosen reactions.



Bi-functional zeolite-encapsulated metal nano-particle catalyst to convert ethane to aromatics such as benzene Toluene and xylenes in one step.

The deactivation challenge in each process and catalyst was different. Thus, the cause of deactivation was attempted to be considered in designing a more active, selective and deactivation-resistant catalyst. This was achieved by for instance addition of second mesoporosity (hierarchical zeolite), zeolite surface modification, metal encapsulation and metal stabilization using sulfur. As a result, catalytic performance including selectivity towards desired products, conversion and life-time were improved for the developed catalysts.

In summary, this thesis offers promising solutions for catalyst deactivation by designing novel catalysts for three important processes that potentially provide more environmentally friendly approach for production of fuels and energy.

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PhD

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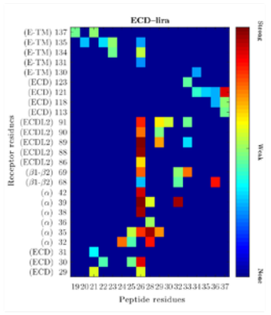
Solution structure of glucagon-like peptide-1 analogues and their interactions with the endogenous receptor and albumin

Since the beginning of the 20th century, the interest for glucagon-like peptide-1 (GLP-1) has been growing. Firstly, due to GLP-1's ability to regulate insulin secretion, and recently, due to its promising properties in treating obesity, preventing cardiovascular diseases, and possibly even dementia. However, it quickly became clear that GLP-1 cannot be administered as a drug, since its half-life in the body is very short. In fact, it is cleared already within a few minutes, preventing its usage as a drug without remedying modifications. Several strategies have been developed to successfully prolong the half-life of GLP-1. One solution consists of attaching a fatty acid (FA) chain to GLP-1. This is believed to cause interactions with human serum albumin (HSA), a carrier protein in the blood, as well as oligomerisation. However, it is vital that the biological function of GLP-1 is maintained.

In this study, the half-life extending properties of different attached FAs were investigated experimentally. The results show that longer FA chains lead to larger oligomers, and that the addition of a charged linker between GLP-1 and the FA chain leads to more stable, but smaller oligomers. In relation to HSA interactions, it was shown that attaching medium to long FA chains cause full interaction with HSA, whereas if there is a linker in between the long FA chains and GLP-1, only partial HSA interaction is observed. This concludes that longer FA chains should increase the half-life. But what about the biological effect? This was investigated using computer simulations, and the results indicate that the effect depends on the site of FA attachment. Furthermore, longer FA chains seemed to be more effective, which goes well with the half-life extension possibly being more pronounced for longer FA chains.

In addition, the pewrformed investigations, using a combination of experimental studies and computer simulations, could provide intel on a level that is very difficult to obtain using only one of the methods. Therefore, the results of this study also present themselves as a methodology for facilitating atomic level investigations of peptide drugs.



Interaction strength between peptide and receptor extracellular domain.

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Characterization of Protein-Excipient Interactions and Protein-Protein Interactions on the Molecular Level Using In-Silico Simulation

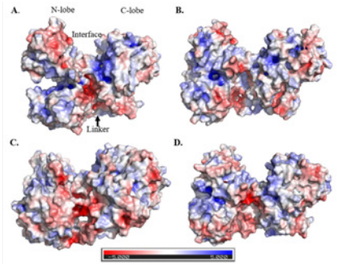
Protein and peptide therapeutics (PPTs), also called biologics, are often characterized by high specificity and potency with low toxicity and has therefore interested many pharmaceutical industries wanting to develop medicines to treat severe human diseases.

As a part of the consortium Protein-excipient Interactions and Protein-Protein Interactions in formulation (PIPPI) this PhD thesis describes fundamental research carried out to investigate the effect of pH and varying concentrations of different additives on diverse classes of PPTs. In the class of peptides, the wild-type plectasin – known as cysteine stabilized antimicrobial defensing – and three variants were investigated using molecular dynamics (MD) simulations in combination with microscale thermophoresis (MST) and nuclear magnetic resonance (NMR).

All the plectasin variants were conformationally stable during the course of 100 ns MD simulations at all pH and salt conditions. However, flexibility in the loop containing a distinct anionic tetrapeptide stretch close to the N-terminus increases with pH due to the change in electrostatics. The conformational stability of the plectasin variants are attributed to the presence of three cystines. Therefore, thermodynamic integration MD simulations supplemented with NMR chemical shift assays were used to determine the order of cystines reduction.

Peptide-excipient interaction hotspots were deduced from MD simulations in combination with MST and NMR measurements. In the classes of proteins, conformational stability of human serum transferrin (Tf) and conjugate fusion protein human serum albumin–neprilysin (HSA-NEP) were examined by combining small angle X-ray scattering (SAXS) and MD simulations in various formulation conditions.

The research findings presented in this thesis indicate the usefulness of combining in-silico and experimental techniques and that this approach can aid in designing new strategies for the formulation of biologics.



Electrostatic potential surfaces calculated for A. PO, pH 5; B. HO, pH 5; C. PO, pH 6.5; D. HO, pH 6.5.

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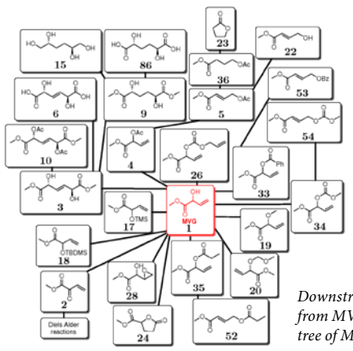
New polymer building blocks from bio-based methyl vinyl glycolate

Methyl vinyl glycolate (MVG) is a chemical compound that can be produced in bulk through a catalytic process from carbohydrates. MVG (also called methyl 2-hydroxybut-3-enoate) is thus a new substance in the series of bio-derived and renewable compounds that can help to reduce the dependence on chemicals from the petrochemical industry and thereby contribute to the climate change mitigation. This is particularly relevant in the production of polymers, the vast majority of which are still produced from oil-based products. The thesis describes the transformation of MVG into a number of new compounds that have potential as building blocks for the production of polymers.

The reactions involve the alkene and the alcohol in MVG, both of which are reactive functional groups for different transformations. The alkene has been reacted in a metathesis reaction, an epoxidation, a cyclocarbonylation and an allylic rearrangement, the latter having been studied in detail with a palladium catalyst to understand the mechanism. The alcohol has been reacted with various electrophiles to form ethers, esters and carbonates. In addition, the alcohol has been oxidized under mild conditions to the corresponding ketone, which is a very unusual and reactive molecule.

The ketone of MVG reacts readily in a Diels-Alder reaction with dienes, thus forming new carbocyclic compounds. A number of these reactions with MVG have been carried out on a large scale, and the compounds have then been investigated as monomers for the preparation of polymers by copolymerization with various reactive substrates. This diverse set of products may support the implementation of MVG on the marked as an alternative to petrochemicals.



Downstream products from MVG, the value tree of MVG.

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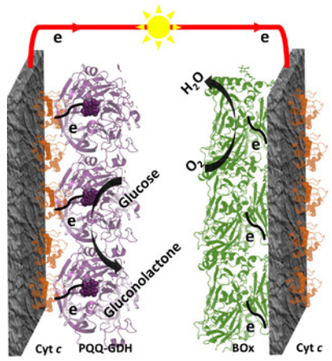
Esben Taarning

Enzymatic Biofuel Cells and Biosupercapacitors: The body itself can drive power supply for miniaturized medical equipment

Miniaturized implantable and self-sustained power supplies for personalized medical devices – based on energy conversion or energy storage – hold significant promise for monitoring and controlling human health and well-being. Biological power sources, such as biofuel cells and biosupercapacitors that can produce electrical power directly from fuels in biological fluids, or store charge using biodegradable catalysts (e.g. enzymes), have therefore attracted great interest.

The aim of this Ph.D. project is to fabricate novel type biological power sources using enzymes or proteins to convert chemical energy to electrical energy or to store electrical charge. The core redox enzyme pyrroloquinoline quinone dependent glucose dehydrogenase (glucose oxidization) and the copper enzyme bilirubin oxidase (dioxygen reduction) were chosen as target enzymes. The enzymes were immobilized on paper electrodes prepared from the conducting 2D-material graphene as anode and cathode, respectively. Combining the two enzyme electrodes into an electrical circuit with fuel supply directly from the body's own liquids then enables generating electricity as an enzymatic biofuel cell. Further integrating the redox protein cytochrome c on both electrodes as a charge-storing component, a fully operating self-charging biosupercapacitor was fabricated.



Schematic representation of the assembled ESBC. The structures of cyt c (rust red), PQQ-GDH (purple) and BOx (green) correspond to PDB 1hrc, 1c9u and 2xll, respectively. Not drawn to scale.

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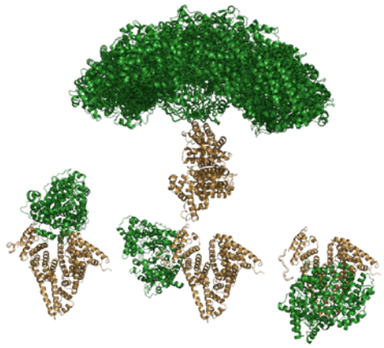
Characterization and solution structure of multi-domain proteins and protein complexes

Protein-based therapeutics have become an essential part of medical treatment. Despite all the advantages of protein-drugs, their stabilization is challenging. Under inappropriate conditions, they might lose their activity and induce severe adverse effects. Stabilization and formulation of protein-drugs is one of the most critical, time-consuming and expensive steps in drug development. Many promising protein-drugs have failed clinical trials due to their stability challenges. Unfortunately, no general rules for the formulation process have been reported and it is not yet possible to predict the behavior of different proteins under different conditions.

This Ph.D. thesis is a part of the Protein-excipient Interactions and Protein-Protein Interactions (PIPPI) project, which goal is to improve the molecular understanding behind protein stabilization and thereby aid the formulation process. The focus of the PhD work is investigation of the stability of three different types of multidomain proteins: transferrin, albumin-neprilysin fusion protein, and monoclonal antibodies. All of them were systematically studied under different physicochemical conditions using high-throughput techniques. These studies were used to choose conditions for structural investigations using small angle X-ray scattering. The results were combined with in-silico methods, such as MD simulation to provide a better understanding of stability on the molecular level. Despite the common trends in stability, all studied multidomain proteins show different behaviors, which can be explained from the molecular structures and interactions. Additionally, the dissertation shows that a combination of multiple methods leads to a better understanding of protein stability.



Different molecular conformations of albumin-neprilysin fusion protein.

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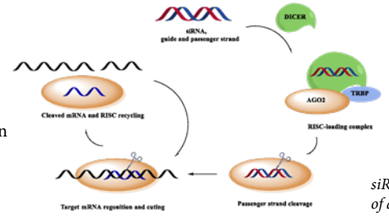
Novel tools for ultra-specific targeting of nucleic acids

Short synthetic oligonucleotides are valuable tools as they find applications in numerous fields including nanotechnology, molecular biology, biotechnology, and clinical diagnostics. From a chemical standpoint, oligonucleotides are polymers built of four nucleotide molecules abbreviated A, T, C and G in deoxyribonucleic acid (DNA), and A, U, C and G in ribonucleic acid (RNA). Oligonucleotide probes can be designed to target any desired part of genome, using a fundamental Watson-Crick base-pairing rule, which is A binds T/U and C binds G. However, translation from bench side to practical applications requires the development of chemically modified oligonucleotide sequences that are gene specific, chemically, enzymatically stable, and efficiently internalized by target cells.

This PhD study focuses on synthesis and characterization of new modified oligonucleotides as potent diagnostic and therapeutic candidates. The project contributes with several modifications that improve properties of short synthetic oligonucleotides. Given a broad applicability of DNA and RNA analogues, this work might contribute to advanced diagnostic and therapeutic tools.

First, the study includes synthesis of a small library of peptide-oligonucleotide conjugates (POCs) and investigation of their biophysical properties. The findings confirmed the POCs ability for efficient target binding and single nucleotide polymorphism (SNP) discrimination. Additionally, the serum stability studies confirmed higher stability of the POCs when compared with the naked-parent oligonucleotides. Finally, the research formulated complexed and conjugated oligonucleotide therapeutics with peptide sequences, designed to reduce the HIV1-mRNA or the BGas lnRNA expression and function. The cell culture experiments showed promising effect and cell internalization for the complexes and conjugates. Nevertheless, the variability within the quantitative results was high.

In addition, a part of this PhD study concentrates on the synthesis of multi-fluorophore labelled oligo-nucleotides for detection of mutated human genes.



siRNA mechanism of action.

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Femtochemistry and Laser Control of Photochemical Reactions

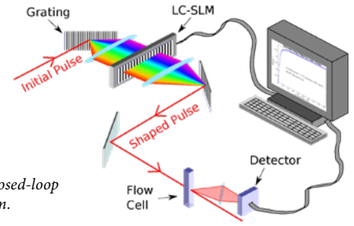
The transformation of one set of chemical substances (reactants) to another (products) is of fundamental importance for chemistry and biology. In a crude manner, traditional means as heat and light (i.e., temperature and frequency of photons) have been employed for decades to guide the reactants into particular product channels.

The atomic-scale dynamics of molecules and chemical reactions unfolds on the femtosecond (10-15 s) timescale and is governed by the principles of quantum mechanics. These principles appear to offer the promise of a vastly improved performance over what is achievable within the classical framework of so-called incoherent processes. To that end, photochemistry with coherent laser light is a potential quantum technology that is a potentially attractive alternative to classical photochemistry.

The PhD thesis investigates the interaction between laser light and molecules in the regime of the so-called non-resonant dynamic Stark effect. This amounts to a time-dependent modification of the interaction potential determined by the pulse envelope of laser pulses and independent of laser frequency. The lack of frequency dependence is a very convenient feature for experimental implementations.

Through theory and computations, it is demonstrated how molecules can be rotationally and vibrationally excited. In a collaboration with an experimental group, the field-free rotational motion of I2 is analyzed. The experimental observations show clear signatures of so-called quadrupole coupling to the nuclear spin states and all features of this coupling are completely accounted for.

It is also shown how laser light can be used in optical purification of a racemic mixture which is a 50/50 mixture of enantiomers, i.e., molecules which are each other's mirror images. In order to close the gap between theory and experiment, the optimized laser-light pulses are constructed in similar way as in pulse shapers that are used in experimental setups.



Sketch of a closed-loop control system.

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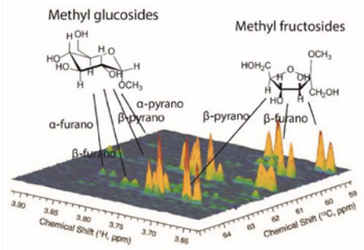
Development of Zeolite Catalysts and Processes for the Selective Conversion of Sugars to Bio-Polymer Monomers

Our current society is highly dependent on non-renewable materials derived from fossil sources, which upon extraction and refining cause net green-house gas emission to the atmosphere, resulting in environmental issues such as climate change. Polymers represent ubiquitous products in daily life and constitute most of synthetic materials. The production of polymers from renewable biomass resources is possible, but technologies are immature for making these bio-based products commercial realities competitive with fossil-based materials.

The thesis explores processes for the conversion of biomass sources with solid zeolite catalysts into chemical building blocks useful for the production of polymeric materials. In particular, different sugars are used as starting substrates. The project also investigates the pathways for the transformation of sugars and the parameters affecting the productivity, achieving deep understanding of the studied reactions and optimized conditions. The parameters for the production of methyl lactate - the monomer of polylactic acid, the most common bio-based biodegradable plastic - starting from common sugars were optimized. Part of the thesis is dedicated to the study of the zeolite catalysts.

The synthesis of the catalytic materials is investigated, and the essential structural properties for obtaining high catalytic activity are elucidated. Finally, the project considers the production of a new bio-based product, methyl vinyl glycolate (MVG), obtainable from glycolaldehyde formed from sugars. The MVG molecule contains functionalities appropriate for representing a building block for the production of new bio-based polymeric materials.

In summary, the thesis provides important insight into existing and new processes for the conversion of renewable sources into chemical products, and conveys useful information for the development of technologies potentially replacing the refining of fossils.



Spectral region of the primary alcohols of 1H-13C HSQC spectra, signals of the different forms of methyl fructosides and methyl glucosides.

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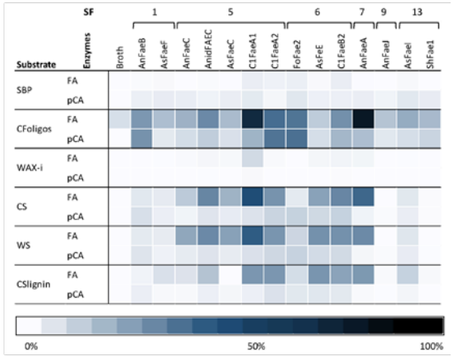
Esben Taarning

Synthesis of biomass-containing xylan fragments and evaluation of ferulic acid esterase activity

Hemicellulose is a collection of polysaccharides with complex structures that together with cellulose and lignin constitute the major constituent of biomass (lignocellulose). The complex structure of hemicellulose makes it difficult for enzymes to degrade biomass, which is viewed as an important and CO_2 neutral energy source if properly utilized.

The thesis first describes the synthesis of arabino- and glucuronoxylan fragments found in hemicellulose. These are of great interest as it is valuable to have access to pure and well-defined fragments of hemicellulose that can be used as substrates for hemicellulose-degrading enzymes such as xylanases, arabinosidases and glucuronidases. The synthesized fragments consist of composite xylose units to which either arabinose or glucuronic acid are bound. First, the xylose units have been assembled into either tetra- or pentasaccharides using a selective coupling method that allows the coupling of two thioglycosides with one another. Next, arabinose units have been loaded onto the tetrasaccharides, while the pentaxylan has been coupled to two different glucuronic acid units, giving a total of five synthetically made xylan fragments. Going forward, removal of the protecting groups will yield the desired fragments that can be used to characterize hemicellulose enzymes.

Another project in the dissertation was completed during an external stay at Wageningen University and Research. Here, work has been done on the characterization of ferulic acid esterases, which form an important part of the arsenal of hemicellulose-degrading enzymes, as these can cleave the ester bond between ferulic acid and polysaccharides. Thus, these enzymes may reduce some of the complexity of the hemicellulose structure. However, these enzymes show considerable differences in reactivity and specificity, which is why it has been investigated whether a previously published classification based on the genomes can be related to the specific reactivity. This was investigated via the release of ferulic acid and diferulic acids from several different types of natural biomass substrates. This showed that two classes of enzymes in particular were very active.



Heatmap for the release of FA and pCA from the natural substrates tested, the results are shown as percentages of bound content (0 – 100 %) as measured by UHPLC-UV. CS: corn stover; WS: wheat straw.

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Master Theses 2019

Ahmad Kasem Haidar
Synthesis of analogues of a lead compound with anti-seizure activity

Alejandro Ventura-Traveset I Julve
In vitro activity of GPCR modulators

Alessio Radaelli
Strain-Release Driven Cycloadditions

Ana Laura Rodrigues da Silva
Fragment-based Drug Discovery

Beatrice Flohr Schultz
Kinetic characterization of TPH1 variants combined with molecular dynamics simulations

Caroline Grønbech Hansen
Analysis of natural products from the fish killing microalgae Prymnesium polylepis and Karlodinium armiger

Christina Sophie Haxvig
Advanced linker technologies for antibody-drug conjugates

Christine Thue Poulsen
Synthesis of a natural product-derived compound collection

Ida Marie Vedel
Kinetic characterization of tryptophan hydroxylase isoforms

Jesper Uhd
Sequence-dependent conjugation strategy for site-selective protein modification

Jonas Himmelstrup
Development and Study of New Reactions with Homogeneous Metal Catalysis

Josefine Hvarregaard Andersen
Derivation and implementation of coupled cluster linear response in the molecular-orbital-based coupled cluster code eT

Kasper Alexander Brauner Hansen
Hydroformylation in gas-phase with supported ionic liquid phase (SILP) catalyst systems

Kasper Juul Møller
Validation of ICP-OES method for assay of pharmaceutical raw material

Kianoosh Moeini
Geothermal Energy Production and Heat Storage Potential of Frederikshavn Formation

Kitti Szabo
Design and synthesis of novel GLP1 variants

Lasse Johansen
Iron-Catalyzed Dehydrogenation of Alcohols

Mette Elmegaard Andersen
Development of New Reactions with Homogeneous Metal Catalysis

Mette Eybye Lindén
Investigation of the ability of acylated peptides to oligomerize and to bind to human serum albumin

Mikkel Rytter Ottosen
Chemoenzymatic Dynamic Kinetic Resolution of 2-Functionalized Aldehydes'

Nikolaos Dimitrios Psaraftis
Novel gene therapeutic for treatment of Dementia with Levy Bodies

Oliver Sørensen Siig
Computational studies of the reactivity of different sites in a deNOx catalyst

Rasmus Lykke Mortensen
Synthesis, Characterization, and Testing of Novel Cross-Linked Polystyrene Materials for Catalytic Hydrogenation of CO_2 to Formic Acid

Stanislav Molodtsov
Synthesis of nickel nanoclusters in zeolites for application as heterogeneous catalysis in the MTG reaction

Tine Marianne Duus
Sequence-dependent conjugation strategy for site-selective protein modification

Umar Fayyaz
Investigation of the effect of electrolyte activities on the recovery of oil in chalk by imbibition

Yemily Luciana Mouret
Hydraulic fracturing in chalk reservoirs under variable stresses

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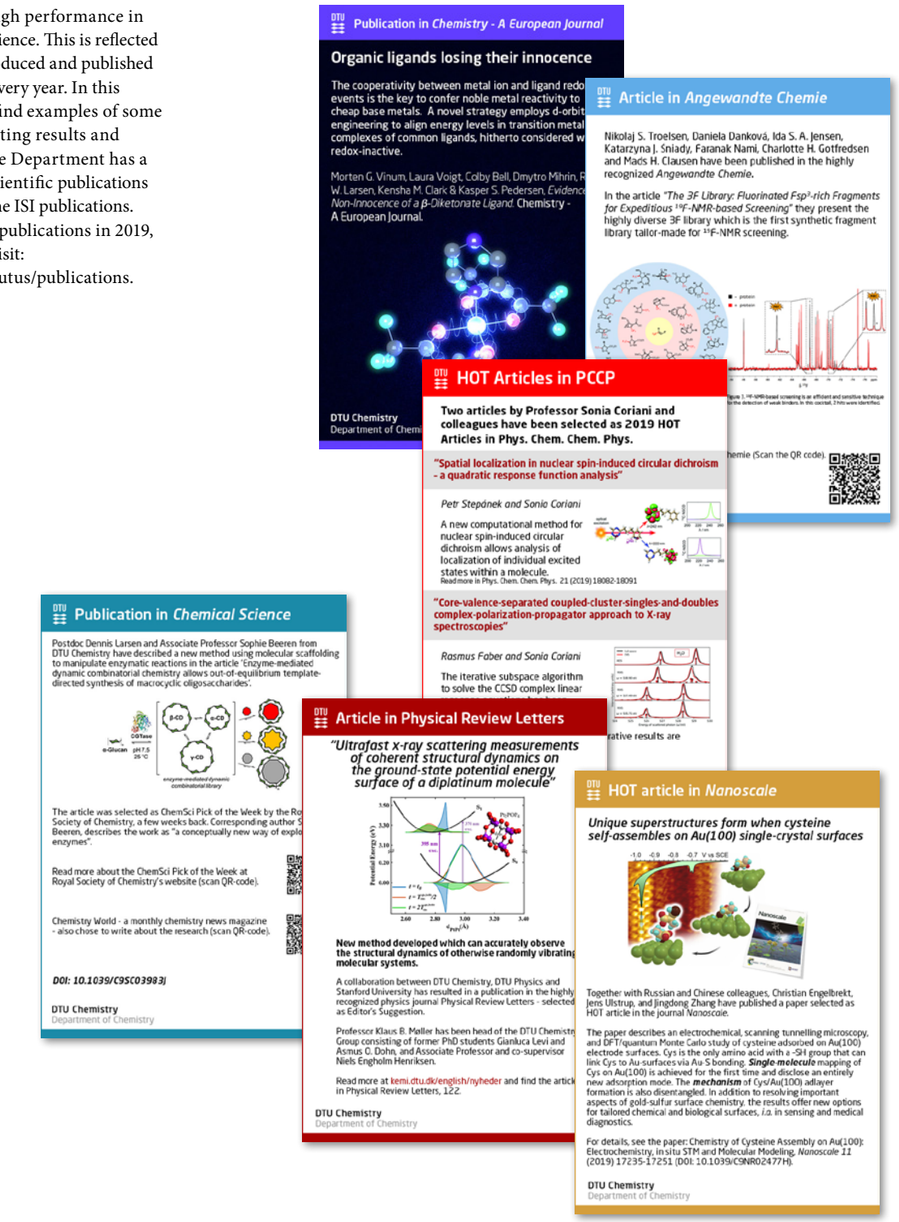
Find DTU Chemistry Students at: facebook.com/DTUChemistryStudents
For more information: Teaching Administrator Mette Christine Møller, mcmo@kemi.dtu.dk

Publications 2019

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 this Annual Report, you can find examples of some of the Department's exciting results and projects during 2019. The Department has a strong track record in scientific publications and we keep increasing the ISI publications.
For a complete list of the publications in 2019, please scan the code or visit:
kemi.dtu.dk/english/aboutus/publications.



Events

Open House

The Department is always very active at DTU's annual Open House event. At the information stands, students, faculty, and Heads of Studies Klaus B. Møller and Mads H. Clausen all answered questions from curious high school students. Around 137 potential students participated in the Chemistry and Technology guided tours, and the effort was not in vain – 88 students were signed up for the BSc programme. Human Life Science Engineering had 68 participants at the guided tours and 60 students signed up for the programme.

Industry Project Day

The Department hosted two Industry Project Days where industrial partners had the opportunity to present potential projects to BSc, BEng, and MSc students from DTU Chemistry. Several companies such as Zealand Pharma, Aquaporin, Novozymes, Haldor Topsoe, and Synopsys Denmark participated with interesting proposals and interacted with the students. Due to the success of the events, more Industry Project Days will be arranged in the future, and DTU Chemistry look forward to seeing even more companies joins.

PhD Symposium

The 2019 edition of the PhD Symposium - held at Konventum, Elsinore - was filled with interesting presentations and posters. Head of Department Erling H. Stenby presented two awards during the symposium: Natalia Teresa Skawinska won 'Best Oral Presentation' for her presentation of "Towards the structure of human tryptophan hydroxylase isoform 2" and Laura Voigt won 'Best Poster Presentation' for her poster titled "Low valent metal-organic frameworks".

The Danish Chemistry Olympiad

DTU Chemistry hosted the 4th round of the Danish Chemistry Olympiad. Associate Professor Susanne Mossin and chemistry student Sofie H. Pedersen had put together an exciting programme for the visiting finalists. During the three days at DTU, the students experienced inspiring lectures from several researchers and had theoretical and practical tests. After a selection process, four students represented Denmark at the IChO (International Chemistry Olympiad) in Paris. The team won one gold and three bronze medals.

REACHING OUT 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. In 2019, ScienceShow was busy with 90 shows all over Denmark – mainly entertaining high school and primary school students. The show also performed at big events such as Folkemødet (Denmark's Democratic Festival), Science Expo, and European Science Fair.

High School Lectures

DTU Chemistry hosts a broad range of lectures for high school students. In 2019, 1153 high school students have participated in lectures such as Spectroscopy and Identification of Organic substances.

DTU Chemistry has selected various highlights from 2019 to supplement the articles on pp. 6-15. You can read more at our website kemi.dtu.dk/English/Nyheder, or follow us on linkedin.com/company/dtu-kemi.

Highlights

GRANTS & HONOURS

The Novo Nordisk Foundation

Professor Mads H. Clausen and co-applicant Assistant Professor Luca Laraia was awarded 10.6 MDKK by the Novo Nordisk Foundation for establishing a new research infrastructure called DTU-ScreeningCore. The aim of DTU-SCore is to provide extensive small molecule screening capabilities for biochemical and cellular assays. The core facility will be a unique high-throughput screening platform at a Danish university and will be open access with a mission to advance biomedical research, serving as a starting point for chemical biology research and early drug discovery. The platform will integrate with the current DK-OPENSCREEN infrastructure and e.g. offer automation for liquid and plate handling. According to Professor Mads H. Clausen DTU-SCore will perform its first demonstration projects in 2021.

Assistant Professor Luca Laraia also received 2.1 MDKK for the research project 'Blocking cholesterol production through specific protein degradation'. Diseases originating from the mis-regulation of cholesterol homeostasis are a significant burden on society. Although statins are widely used to lower blood cholesterol levels, their extended use can result in overexpression of their target protein HMG-CoA reductase (HMGR), in a compensatory mechanism. By using the recently developed strategy termed proteolysis targeting chimera (PROTAC), the Laraia Lab aims to design ligands of cholesterol biosynthetic enzymes that cause protein degradation, rather than inhibition.

The Novo Nordisk Foundation granted Associate Professor Sophie Beeren 2.87 MDKK for a research project that combines enzymology with supramolecular chemistry. She will exploit enzymes to catalyse the reversible formation of glycosidic linkages between unprotected monosaccharides and generate dynamic mixtures of oligo-saccharides under thermodynamic control. Ultimately, this will make industrial production methods more sustainable by reducing the emission of greenhouse gases and lowering energy and water usage, because enzymatic processes are fast, specific and take place under mild conditions in water.

The Carlsberg Foundation

Associate Professor Sophie Beeren received 4.5 MDKK from the Carlsberg Foundation: Young Researcher Fellowship for her research in sustainable enzymatic processes.

The Carlsberg Foundation has also awarded three researchers with infrastructure grants. Associate Professor Susanne Mossin received 250,000 DKK for a mass spectrometer for operando spectroscopy – enabling simultaneous evaluation of both structure and activity of e.g. a catalyst in action. The second recipient, Assistant Professor Luca Laraia, was granted 190,000 DKK for a state-of-the-art imaging system for chemical biology. Finally, the Carlsberg Foundation awarded Professor Mads H. Clausen 734,900 DKK to support the new aforementioned DTU SCore infrastructure.

Independent Research Fund Denmark

Professor Robert Madsen has been awarded 2.88 MDKK from the Independent Research Fund Denmark for developing 'Chromium-Catalyzed (De)Hydrogenation Reactions'. Reactions with hydrogen gas constitute the most important catalytic transformations in organic chemistry. Unfortunately, homogeneous catalysts for these transformations are based on precious platinum group metals or other expensive metal complexes. In this project, inexpensive and non-toxic chromium catalysts will be developed for the dehydrogenation of alcohols and the hydrogenation of unsaturated functional groups.

In another project, Mads H. Clausen aims to develop new glycan-based cancer vaccine candidates for improved immunotherapy, which the Independent Research Fund Denmark chose to grant 2.4 MDKK. Immunotherapy is currently revolutionizing cancer therapy by harnessing the power of the immune system against cancer cells. The identification of tumour associated carbohydrate antigens (TACAs), aberrant types of glycans decorating tumour cells, has paved the way for the development of cancer vaccines. Based on the hypothesis that fully glycan based cancer vaccines can represent a way to improve active cancer immunotherapy, the research approach will include the preparation of vaccine candidates based on ganglioside TACAs that are easy to formulate and able to elicit an immune response independent from individual polymorphisms.

Assistant Professor Luca Laraia received two large grants from the Independent Research Fund Denmark. The first project was awarded 2.87 MDKK and aims to develop a general approach to identify oxysterol-interacting proteins by combining induced protein degradation with high resolution, proteome-wide mass spectrometry. The second project 'Unravelling the sterol-interacting proteome using limited proteolysis small molecule' was granted 2.87 MDKK.

EU Horizon 2020

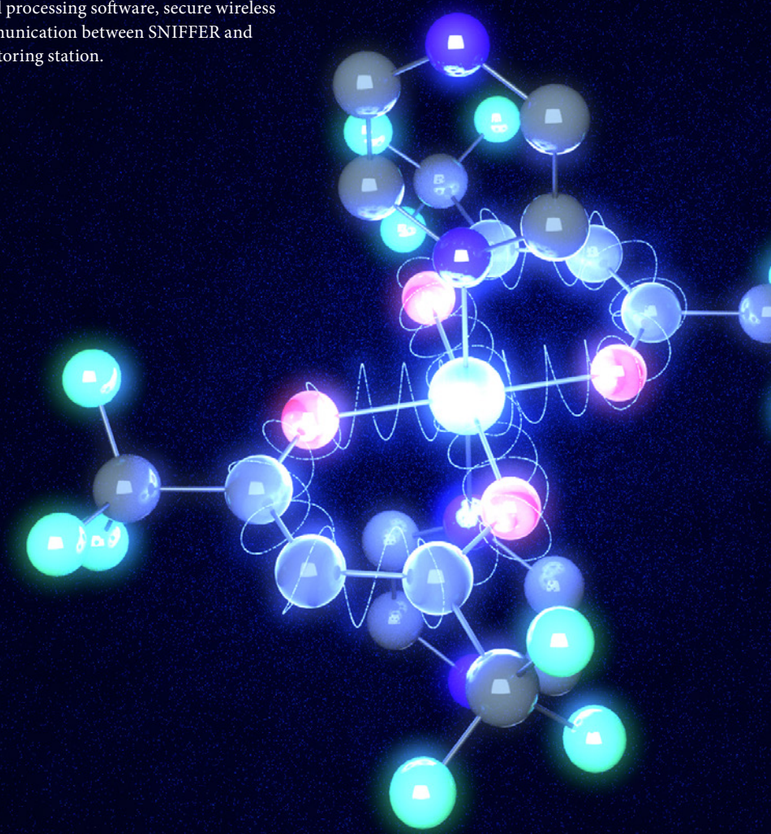
Professor Anders Riisager, MACBETH consortium partner from DTU Chemistry, has received 5.2 MDKK from EU Horizon 2020 under the grant type SPIRE – Industrial Sustainability. The MACBETH consortium provides a breakthrough technology for advanced downstream processing by combining catalytic synthesis with the corresponding separation units in a single highly efficient catalytic membrane reactor (CMR). This disruptive technology has the ability to e.g. reduce greenhouse gas emissions of large volume industrial process by up to 45 % and will be further developed in this project. The MACBETH consortium consists of 25 partners, with Evonik Performance Materials as consortium lead.

Anders Riisager has also received 4.44 MDKK for a future Marie Skłodowska-Curie Innovative Training Network called Coordination Chemistry Inspires Molecular Catalysis (CCIMC EJD). The network addresses the current lack of coordinated doctoral training at the European level on molecular catalysis. It aims to push the frontiers of knowledge in ligand design, coordination chemistry, precatalyst development, catalyst recovery and catalytic process implementation, while also offering full scale training in professional and personal transferable skills, to prepare a new generation of junior scientists to meet the economic and societal challenges of the chemical industry in the 21st century. To achieve these objectives, a consortium of 9 academic beneficiaries from 7 European countries will recruit 15 doctoral students to work on coordinated projects in close cooperation with the industrial sector.

Postdoc Cecilia Romano was awarded a 1.55 MDKK Marie Skłodowska-Curie Individual Fellowship for her research within ARGONAUT: from the synthesis of gAnglioside tumouR antiGens to a platfOrm for caNcer Active.

The Danish Ministry of Defence

Associate Professor Mogens Havsteen Jakobsen received 2.47 MDKK from the Danish Ministry of Defence for 'portable SNIFFER detection of improvised explosives. The overall objective of the project is to make the world a safer place for the public, by developing an easy to use handheld detector, wwhich can detect improvised explosives and precursors. The portable SNIFFER will detect improvised explosives and precursors for improvised explosives. The sniffer system includes the following components: Air sampling, Sensor system with colorimetric chip cassettes, Monitoring station with signal processing software, secure wireless communication between SNIFFER and monitoring station.



Highlights

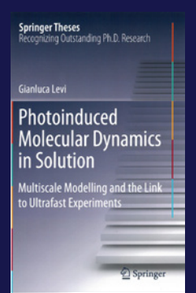
Robert Madsen receives 'Lecturer of the year' award

In order to educate world-class engineers, you need world-class teachers. That is why Polyteknisk Forening annually honors two lecturers as 'Lecturer of the Year', and in 2019, Professor Robert Madsen from DTU Chemistry was one of the recipients of the distinguished honor. Robert Madsen has – among other courses –taught the introductory courses in organic chemistry for almost 20 years.

OTHER GRANTS AND HONOURS

Internationally top-ranked research institutes annually select their best PhD thesis for publication in the scientific portfolio series 'Springer Theses'. In 2019, the theses of Gianluca Levi and Duncan Paterson from DTU Chemistry was selected. Gianluca Levi for his work on 'Photoinduced Molecular Dynamics in Solution' and Duncan Paterson for 'Flash Computation and EoS Modelling for Compositional Thermal Simulation of Flow in Porous Media'.

Two talented master students, Helena Damtoft Tjørnelund and Tobias Nørby Hansen, have been selected to receive the Novo Nordisk Foundation scholarship, which is awarded to the country's most talented master students in the natural sciences. Both will be awarded 35,000 DKK – enabling them to focus 100 percent on their theses.



Lecturer of the Year 2019: Professor Robert Madsen from DTU Chemistry.

Photo: Ulrik Jantzen

Key numbers

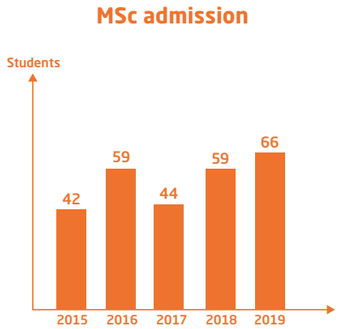
A Leading Research Department

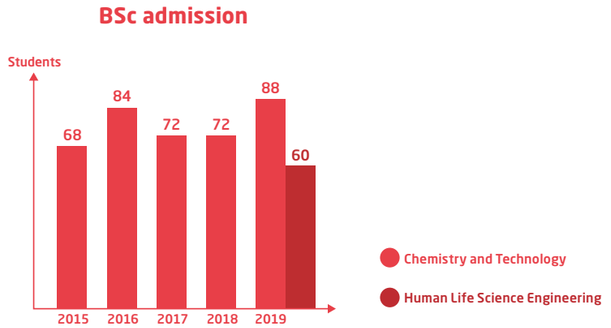
DTU Chemistry focuses on scientific excellence through people, projects, and results in order to remain a leading research department. The Department had a high success rate in applications for external funding in 2019. We are pleased to find that sources outside DTU such as public funds, private companies, and private foundations take increasing interest in the activities at DTU Chemistry.

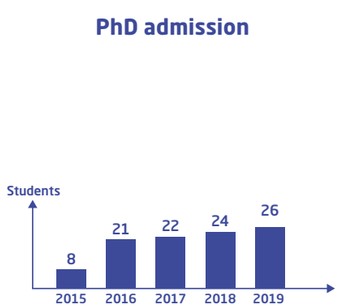
DTU Chemistry is still very successful in attracting scientific talent. We have in recent years had a consistent high number of applicants for the BSc in Chemistry and Technology. Accordingly, DTU Chemistry recently expanded the number of applicants we can accept from 72 to 88.

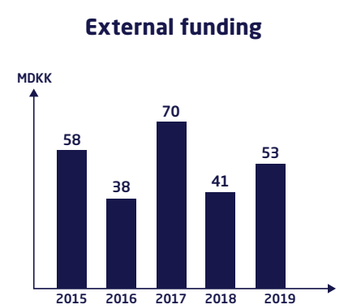
The MSc programme in Applied Chemistry also expanded in 2019. Just like Chemistry and Technology, Human Life Science Engineering with Professor Mads H. Clausen as Head of Studies is a popular choice for the bright, future scientists.

Our research groups are flourishing with new PhD talent. Once again, the Department hired a record number of PhD students in 2019.









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Obituary for Professor Jingdong Zhang

On Thursday, 9 January 2020, Professor Jingdong Zhang passed away after a long period of serious illness. Jingdong's death is a huge loss for her family, colleagues, and students at DTU Chemistry. She was just 51 years old.

In the later 20th century, electrochemistry underwent a renaissance by introducing new methods of solid-state and surface physics, not least due to scanning tunneling and atomic force microscopy. Professor Jingdong Zhang mastered "the new electrochemistry". Over the years with Jingdong as a strong driving force, her group at DTU Chemistry developed the entirely new concept "Single-molecule Electrochemistry of complex molecules and biomolecules", now broadly adopted by research groups in Europe and the USA.

Six or seven years ago, Jingdong launched a new research program, "Untraditional Nanomaterials in Electrochemistry and Bioelectrochemistry", focused on electrochemical surfaces of graphene, metallic nanoparticles and their combinations. She progressed very far in combining this new materials science with electrochemistry of both enzymes and entire bacterial cells, even constructing working bio-electrochemical sensors and bio-fuel cells.

Until the very end, Jingdong was an extremely active and inspiring supervisor and an accomplished and well-liked lecturer in our undergraduate courses. As you approached her classrooms, you would always be delighted to hear her enthusiastic teaching style.

Professor Jingdong Zhang will be missed by us all.

Jens Øllgaard Duus,
Erling Halfdan Stenby,
and Jens Ulstrup

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Jingdong Zhang

1992 MSc in applied chemistry from Shanghai University
1996 PhD in analytical chemistry from Changchun Institute of Applied Chemistry
2016: Professor of inorganic chemistry at DTU Chemistry.

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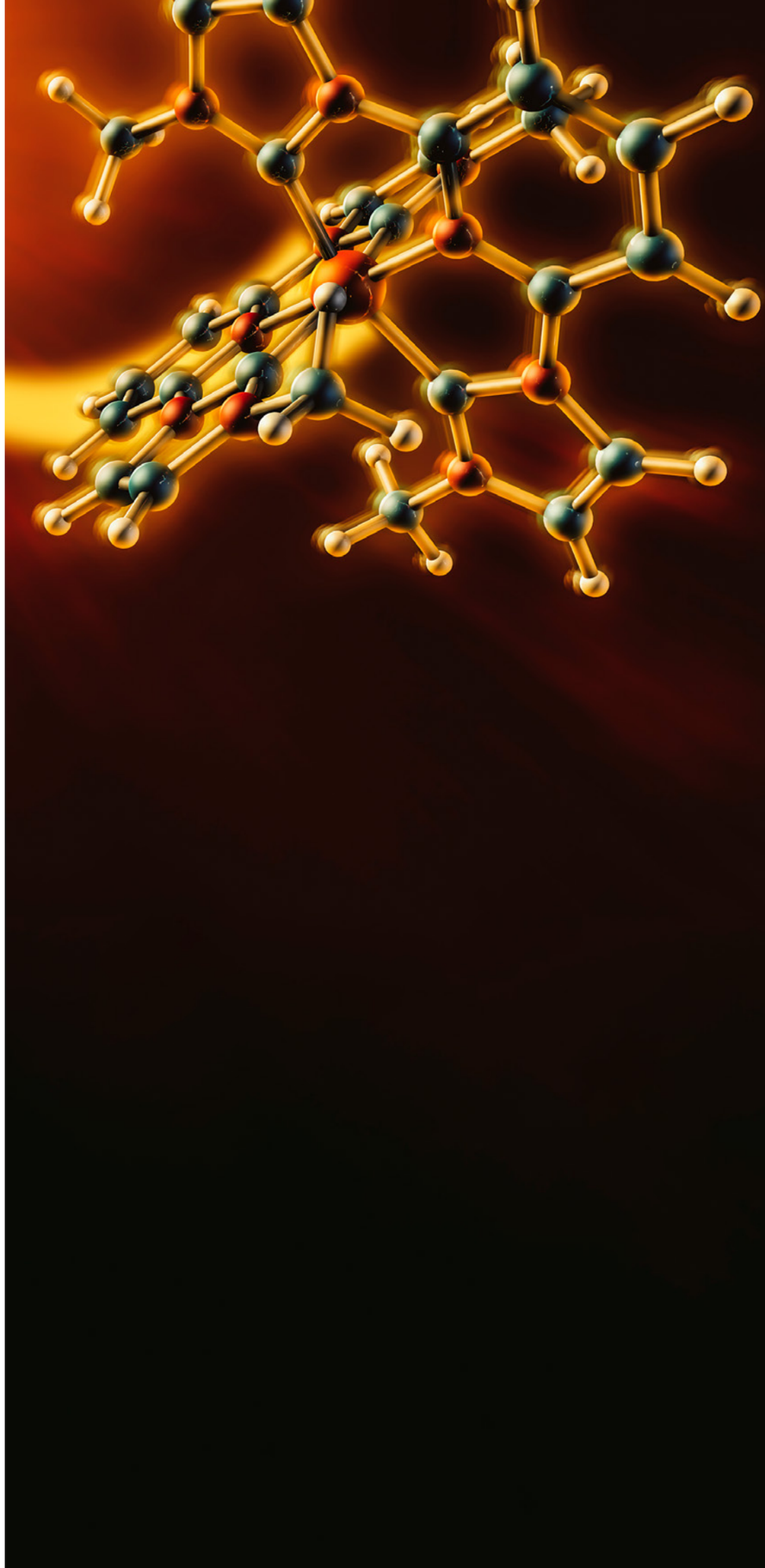

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Annual Report 2019

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