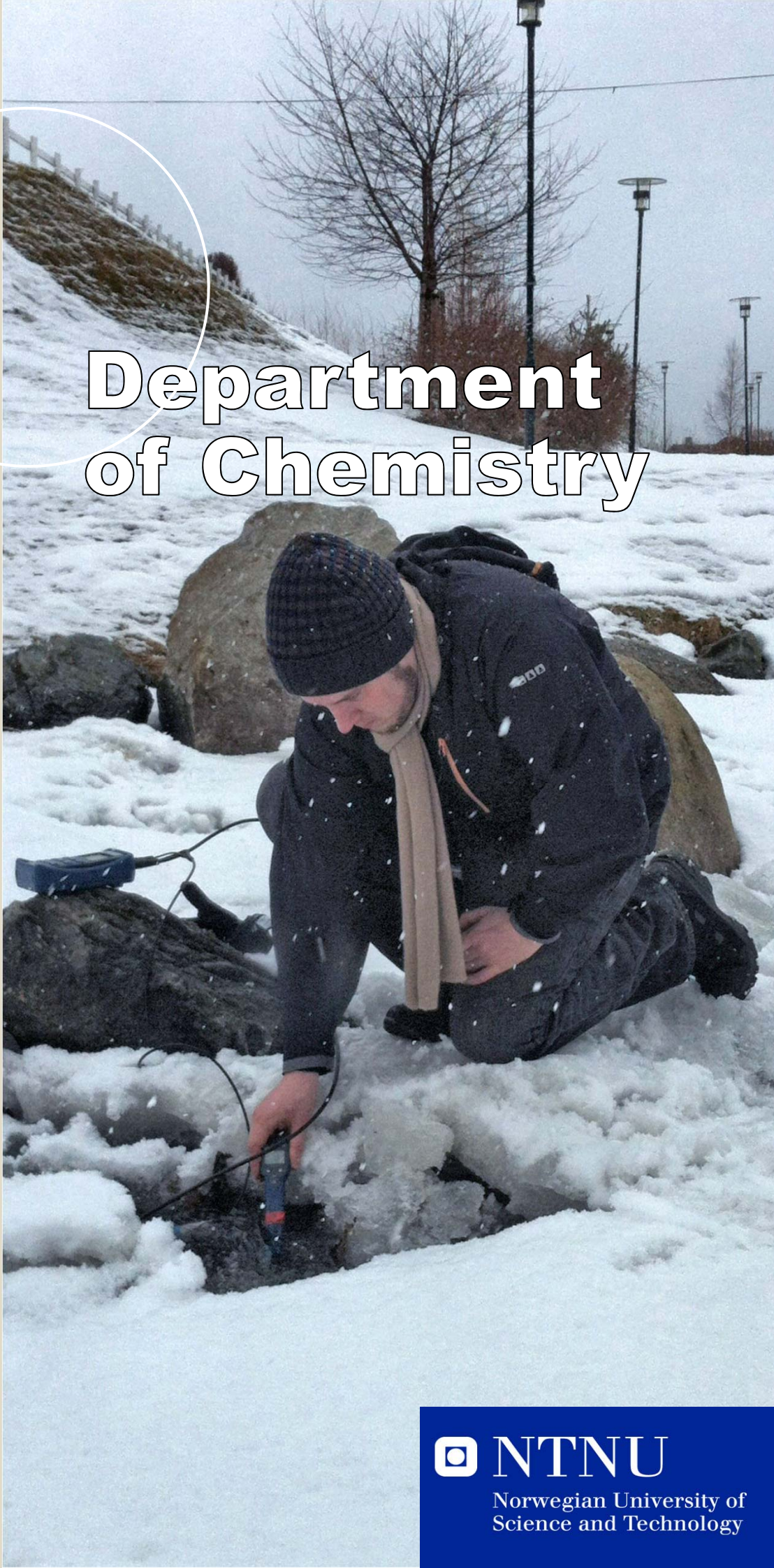
Department of Chemistry

Annual Report 2012



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COVER PAGE

Collecting samples from Ilabekken (The Ila stream). Students are monitoring the stream of content of organic matter and trace metals by the KJ2073 course.

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The department of chemistry

A glance at 2012

During 2012, the Department of Chemistry welcomed two new faculty members, associate professors Murat van Ardelan and Titus van Erp. They joined respectively the environmental chemistry group and the applied theoretical chemistry group. Assoc. Prof. Murat van Ardelan is a marine biogeochemist. Current research of Murat includes studying the impact of CO2 seepage from storage sites and ocean acidification on biogeochemistry of seawater and sediment-water interface in the benthic system, and the impact of eutrophication to coastal ecosystems. Before joining us, Titus was senior researcher at the Department of Surface Science and Catalysis in Leuven, Belgium. Titus's research aims to bring forward the molecular understanding of complex processes using state-of-the-art simulation techniques. A large part of his research is also devoted to the development of new innovative methodologies that can enhance the accuracy of present methods and expand accessible time- and system scales of computer simulations. The department was in the process to recruit several additional faculty members, presenting a strategic opportunity to enhance its research activities, during the spring 2012 when this process was postponed by the Faculty of Natural Sciences and Technology due to economic reasons.

The Department of Chemistry welcomed as well two adjunct professors in 2012. Fernando Bresme is an associate professor from the Department of Chemistry, Imperial College from London. His activities focus on the development and application of computer simulations to investigate the properties of nanomaterials and biomolecules. Per Johan Brandvik is senior scientist at the Marine Environmental Technology Department from SINTEF Materials and Chemistry.

Excellent student recruitment is one of the department's top priority and we were pleased to welcome four new PhD candidates to the department during 2012: Øivind Wilhelmsen, Emilio Catelli, Mehdi Mahmoodinia and Magnus Waage. The number of PhD students in the department at the end of 2012 counted 34. This is equivalent to 2011. In addition IKJ had the pleasure to welcome Vishwesh Venkatraman as new post-doc in 2012. The number of post-doc in the department at the end of 2012 counted 4. Most of our new PhD candidates are offered a 4 years contract in order to cover our large needs for teaching assistance, especially in the laboratories for our basic courses. One of our main challenges is to recruit sufficient Norwegian speaking candidates since the first years program should be taught in Norwegian.

The number of credited publications in 2012 and in international journals was 61 in so-called level 1 and level 2. This is substantially more compared to the numbers of 2011 when 53 publications were registered.

Increasing the awareness on health, safety and environment is a constant attention at the Department of Chemistry. Many important milestones were achieved in 2011. In 2012, the department has been focusing to sustain a standing and good culture in the laboratories. An important factor in the success of these efforts is the continuous attention from all employees and especially the dedicated efforts from our HSE coordinator. The Department of Chemistry was given credit, for example, to be the only department at the faculty which, by the end of 2012, has managed to handle and close all deviations from the deviations report system. Not mentioning that the Department of Chemistry has been involved within the HSE working group at the faculty since its beginning, contributing to the implementation of the HSE courses for both students and employees among other tasks, a major contribution for the unity at the faculty that we can award to our HSE coordinator, Nina Klausen.

There is a growing pressure on the scientific staff to provide external funding for their activities. The success rate for applications in basic research is low, even for applications receiving excellent reviews. This is mainly due to underfunding of the Free Projects programs from the Research Council of Norway. Nevertheless the level of external funding has increased continuously in the past years for the Department of Chemistry, summing up to 9.15 MNOK in 2012 compared to 7.7 MNOK back in 2009. While this is encouraging, we still have a long way to go to reach our goals. And since the Research Council of Norway is keeping its grant allocation for basic research to a low level, our goals will not be achieved unless the department increases its effort within applied research. Yet, 3 major projects, financed by the Research Council of Norway, were developed in 2012. The first project developed by the applied theoretical group aims to investigate the novel thermal orientation effect, in order to uncover the general rules that control this effect at molecular states. This project combines both theoretical and experimental approaches. The second project, initiated by the same group, aims to develop an existing Norway-China collaboration with the goal to increase the energy efficiency in the industrial sector. The third project, developed by the environmental group, aims to study the roles that atmosphere, aerosols, snow and ground play on the mercury cycle at Ny-Ålesund.
It is important to search for funding sources besides from the Research Council of Norway. Several major projects were a successful in this matter at the Department of Chemistry in 2012. Thus, one major project developed in collaboration with Statoil and the applied theoretical group aims to study the kinetics of gas hydrates, in order to understand the processes of gas exchange and hydrate dissociation. PRESIOUS, a STREP project, was developed in collaboration between the environmental chemistry group and the Department of Computer and Information Science at NTNU. It aims to propose innovative methods and tools to augment the static as well as dynamic geometric data of Cultural Heritage objects.

Due to some staff change in the physical chemistry group, the group took the decision in 2012 to modify their strategy and their name. The main strategy of the group will be to focus and strengthen the research profile in the disciplines of applied theoretical chemistry. Simulations at the atomistic and mesoscopic scales are becoming essential tools in state of the art chemical research and thus the strategic prioritization of theoretical chemistry is in accord with these developments in modern chemistry. The group decided to take the name of: “Applied Theoretical Chemistry”.

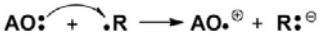
In 2012, the Faculty of Natural Sciences and Technology was granted the funds to purchase 2 new LCMS instruments. This was a main accomplishment for three departments including the Department of Chemistry. 2012 has been busy with the evaluation of the offers from several suppliers, the purchase of the equipment and the installation.

In June 2012, Professor Henrik Koch received the price for outstanding educational activities. In addition, Anette Opsahl, who is a student from associate professor Karina Mathisen, was awarded the price for the best Master Student.

Marie-Laure Olivier
Head of Department

Antioxidants – antireductants

Antioxidants are ingested in increasing amounts since they give the consumer the impression that they are good for them, even they don't know why or how.
Chemists know that antioxidants defang harmful reactive species by electron transfer to pair the lonely electron of a radical:



The antioxidant action of carotenoids is always perceived as an electron transfer to R.
However, scavenging radicals by carotenoids could, in principle, also happen by uptake of the radical's electron. Electron uptake of electrons by carotenoids has so far been enforced by radioactive procedures or metal reactions in vacuum. Christer Øpstad had previously found that this reaction can easily be done on the lab-bench. These investigations were last year systematically extended by *Mohammad Zeeshan* in the lab and by Ana Martinez at the KanBalam supercomputer in Mexico. It was found that the super-antioxidant antaxanthin is not only superior in giving electrons to radicals, astaxanthin can likewise take up electrons and, therefore, act as antireductant. Thus, the superiority of astaxanthin has been substantiated by its ability to give and take electrons in contact with radicals (*Tetrahedron Lett.* 2012, *53,* 4522):

A scientific problem was elucidated, a linguistics problem emerged. The word antireductant does not find grace. Indeed, the word is awkward, but that is the word antioxidant, too. An oxidant removes electrons from a compound, a reductant gives electrons to a compound. Consequently, carotenoids, when giving electrons, should be called reductants, instead they are called antioxidants. The contrary of an antioxidant is an antireductant. The discomfort is additionally increased by calling a compound that attracts electrons prooxidant. We have thus 3 different designations for electron uptake and 3 designations for electron delivery:

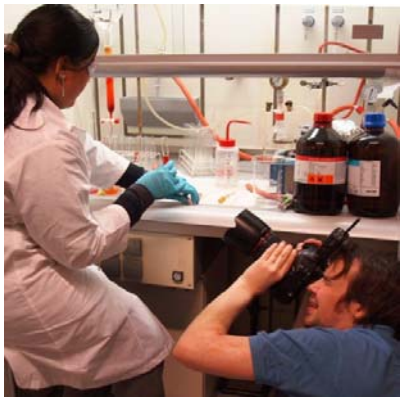
reductant	oxidant
antioxidant	antireductant
proreductant	prooxidant

It is time to put an end to these obscuring terms.

There are several antioxidant actions, the most important are radical scavenging and singlet oxygen quenching. A multitude of antioxidant tests differently define "antioxidant" by specific procedures. Thor Bernt Melø from the Department of Physics had the idea to express the antioxidant activity of carotenoids by a general term, the antioxidant ratio ar, by dividing the reactivity constants for electron transfer (radical scavenging) kel and energy transfer (singlet oxygen quenching) k_{en}.

$$a_r = \frac{k_{el}}{k_{en}}$$

Generally, it is perceived that carotenoids are better antioxidants with an increased number of double bonds. When we measured a series of related carotenoids with different polyene chain lengths, we found that the longer ones are not better. The antioxidant ratio a_r reached an optimum with 11 double bonds, the number found in most natural occurring carotenoids (*Tetrahedron* 2013, *69*, 219).
The longest measured carotenoid in these experiments was synthesized by *Asma Zaidi* and the photographer from the faculty was enthusiastic to detect a colorful motive.



Richard Sliwka, Vassilia Partali

Towards a more resource-efficient society. The concept of exergy.

Introduction

According to the International Energy Agency (2011), it is necessary to increase the energy efficiency in the society at large, in order to avoid a 2 degree rise in average global temperature within 2050 and damaging climate changes. This work addresses some measures that need be taken to realise a substantial increase in the energy efficiency world wide.

There is first a need for consensus on how the energy efficiency should be measured, as several definitions are presently in use. We propose to use systematically the concept of the exergetic efficiency, which measures the use of available work. Exergetic efficiencies can be used to map efficiencies in a society at large. We shall present such a map for Norway, and discuss how it can be used to foster a development towards more resource-efficient technologies. With reference to the situation in Norway, we discuss whether we can expect significant improvements in the way that we produce or consume power. Examples from the offshore-industry and the metallurgical industry are used to illustrate the possibility.

A development towards a more resource-efficient society depends on the availability of highly competent persons in several sectors of the society. Universities should be granted training programs for this purpose.

Defining the energy efficiency

All energy conversion is ruled by the laws of thermodynamics. The first law says that energy is conserved. It is therefore paradoxical to speak of energy consumption. The second law of thermodynamics gives a quality scale for energy, with electric and chemical energy being higher on the scale than thermal energy. By quality we mean the potential to do work. This varies largely among the energy forms. The potential to do work is a quantity known by several names, e.g. ideal or available work or exergy. We shall use the term exergy, (for terminology, see Tsatsaronis, 2007). Exergy can be used to evaluate materials as well as electric power, cf. exergy analysis (Kotas, 1995).

Broadly speaking, we divide definitions of energy efficiency in two categories; those based on the first law of thermodynamics only, and those using both laws of thermodynamics. The definitions related to the first law of thermodynamics consider all energy forms on the same footing. The efficiency measures the useful output energy over the input energy. An efficiency which does not account for energy quality can be misleading about the potential for improvement. Consider as an example the heating of water by the use of electric power (as in an electric kettle). This process has a large first law efficiency, because nearly all electric energy is used to heat the water. But the high quality electric energy, used for simple heating purposes, could have been used to do work.

An efficiency defined from the first and second law of thermodynamics measures the work output with respect to the highest possible work theoretically obtainable, see Kjelstrup et al. (2010). The real process is now compared with an ideal process. In the real process, the exergy leaving a process is always less than the exergy entering a process. This enables one to rank different power producing and consuming technologies by their exergetic efficiency. Work and power have absolute values. They are not conserved quantities like energy. Thus, we can speak of using power.

The difference between the exergy entering and leaving a process is called the lost exergy. To reduce the amount of lost exergy is the way towards a resource efficient society. The exergetic efficiency is the ratio between the exergy output and the exergy input of a process.
A map showing the exergy input and output and the lost exergy, is called a Grassman diagram.

The potential for increasing sector energy efficiencies in Norway

An exergy analysis was carried out for the Norwegian society of 1995 by Ertesvåg and Mielniek (2000), see Fig.1. Exergy streams in the Norwegian society are shown. Similar studies have been done for Sweden, Italy and other countries. Supply and use of exergy have changed since 1995, but the figure is still relevant. The left hand side of the figure gives an overview of the available exergy. Waterfalls represent a large share of the total exergy. Exergy is also available from biomass, oil and gas. Offshore gas- and oil activities are not included. Except from water power, renewable power sources were few in 1995. Wind turbines were only in the planning stage.

The relative contribution of hydroelectric power and oil/gas has since then changed and so have the plans for their use. The large areas of power consumption are shown to the right in the figure. This is what we use the exergy for; production of products from wood, food, light, mechanical work, aluminium and other metals, chemicals, transport or logistics and heating of houses/rooms. The interesting information for each sector is the exergetic efficiency, the ratio between the exergy input and the exergy output, cf. the definition above. We notice large exergy losses. Parts of this exergy could have been used for other purposes.

The figure gives immediately a perspective on where efforts are needed. The transport sector and the domestic sector stand out by having rather low

efficiencies. The first case can be explained by the low efficiency of the combustion engine. The second case is special for Norway; it is due to our use of high quality electric power to heat houses. Much effort has been devoted to increase the efficiency in the transport sector world-wide, but it is still not large. Some effort has been made to improve the way we heat houses in Norway. The government has via ENOVA given support to increase the use of heat pumps. Heating by water from incinerators is also a step in the right direction. The research centre on Zero Emissions Buildings, funded by the Research Council of Norway, is also an answer to this challenge.

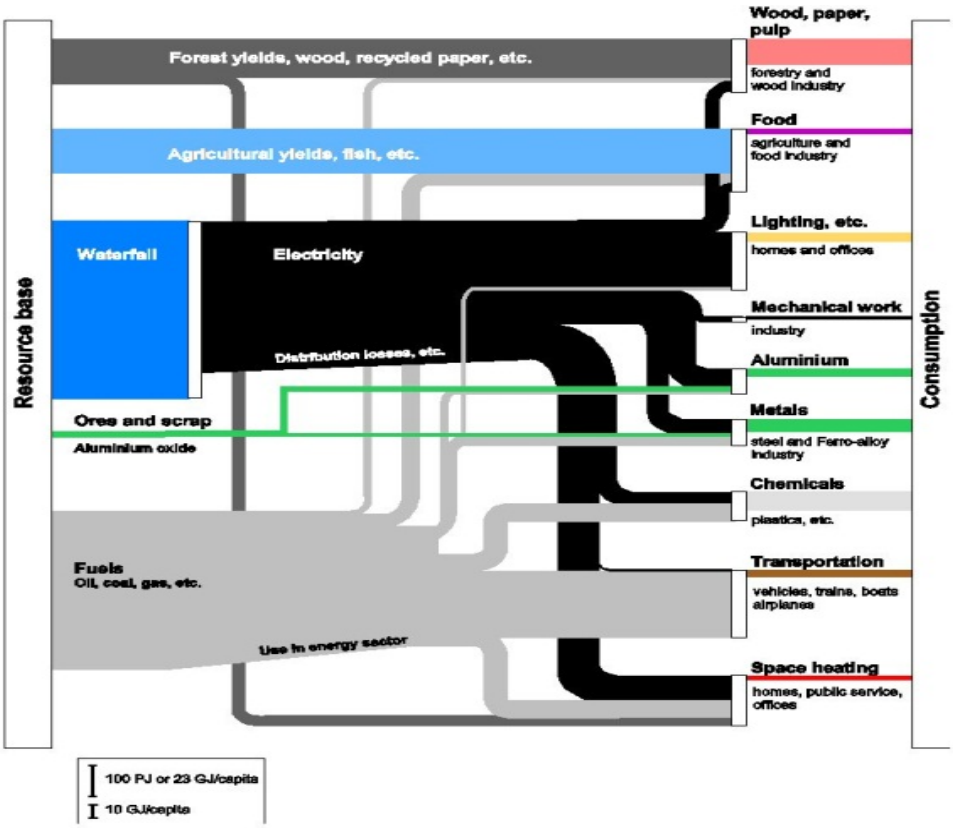


Figure 1. Grassman diagram for the Norwegian society in 1995. Offshore gas- and oil activities are not included. (Ertesvåg and Mielnik, 2000)

In the perspective of the Grassman diagram in Fig. 1, the industry is not an inefficient user of exergy. The sector can however also improve, and exergy calculations can help explain how and how much. The two examples below illustrate the use of exergy calculations in industry. For other examples, see Rian and Ertesvåg (2011, 2012).

Consider first the operation of a typical offshore platform. In 2008, offshore gas turbines and diesel engines were responsible for 21 % of Norway's total CO2 emissions (Statistics Norway, 2010). The exergetic efficiency of oil platforms depend on the modus of operation (Voldsund et al. 2012). The oil and gas separation at a North Sea oil platform was studied for a typical production day in 2011. Parts of the process equipment were designed for a larger volume of gas. In order to deal with this, gas was constantly recycled around several gas compressors. By removing the recycling, the exergetic efficiency increased from 0.32 to 0.38, and the power consumption sank by 3.6 MW (Table 1). The large improvement requires update of some equipment. The results in Table 1 can be used to find out when the update is beneficial.

Exergy calculations can be used to set standards by companies or governments. The exergetic efficiencies for the North Sea process can be compared with efficiencies for production of hydrocarbons from unconventional sources; from Canadian shale fields or from gas hydrates.

	Case1 With gas recyclimg	Case2 Without gas recyclimg
Power consumption / MW	23.9	20.3
Destructed exergy / MW	16.1	12.6
Specific power consumption / kWh/Sm3 oil	180	154
Exergetic efficiency	0.32	0.38

Table 1. Power consumption, destructed exergy, specific power consumption and exergetic efficiency for oil and gas processing at a North Sea platform for a typical production day in 2011 according to Voldsund et al (2012). Results are given with and without recycling of gas.

Consider next the operation of a typical Norwegian silicon smelter which has an exergetic efficiency of 0.31 for typical operating conditions. Table 2 shows that installation of a power producing boiler and steam turbine in the gas outlet section of the furnace can increase the exergetic efficiency from 0.31 to 0.39. This is a substantial improvement (Takla et al., 2012). The numbers can be used to argue that installation of such equipments is important, not only for the single plant, but for all plants. The government can promote a development in the direction of better efficiencies in several ways; by rewarding such changes, or punishing less optimal behaviour.

	Case1 No power recovery	Case2 With power recovery
Exergy in / MW	22.1	22.1
Lost exergy / MW	15.3	13.5
Specific power consumption / kWh/kg Si	11.7	9.6
Exergetic efficiency	0.31	0.39

Table 2. Exergy input, lost exergy, specific power consumption and exergetic efficiency in the case of no recovery and recovery of thermal exergy from the furnace off-gas for one furnace operating at a silicon plant in Norway according to Takla et al (2012). The numbers are scaled to one hour production in a 10 MW furnace. The product includes silicon metal as well as electric power delivered from the energy recovery system. In Case 2, the recovered exergy is used to power the process. The specific power consumption is the power that has to be used beyond this.

In the context of these examples, it is interesting to see a proposal of Sauar (1998) to tax the excess lost work. Such a proposal cannot be realised without knowledge of reasonable values of lost work, however. The theoretical upper limit of the exergetic efficiency is unity, but in practice lower limits apply. The practical limit is specific for each technology, given the operating conditions of the equipments used and the demanded rate of production. Who should define the practical limit? We propose that not only the industry itself should do that. Each user should have to defend their use of quality resources.

Industries are now required in their annual report to give all facts related to their production. With a public demand for quantitative information on the use of exergy sources, each sector of society may need also to document their exergetic efficiency. Such documentations may not only be used to justify the needs of each sector, they may lead to stable long-term framework agreements. The more facts we have on exergy and its use, the more options we have to foster a development towards more environmentally friendly technologies. To understand the optimal operation and the potential for improvements is crucial.

We propose that the Grassman diagram of 1995 for Norway is updated to increase awareness of these matters. As we study the various needs for exergy, as illustrated in Fig. 1, we understand that an overall increase in exergetic efficiency must come, not only from one exergy source, but from all possible sources and uses. The future will see a variety of exergy sources, all tailored for special purposes and needs, taking advantage of local conditions. The potential of ocean power in terms of salt power plants and tidal plants is not yet explored beyond the test stage (Veerman et al. 2009).

A knowledge-based development

The development described above is knowledge-dependent. It requires insight and competence on the highest level, to further develop the most sophisticated parts of our society. In this context, one might first ask; given that we already are so advanced, is there any room for improvement? We can answer this question in detail by studying the single process, but also in a broad manner by looking at the curve in Fig. 2 calculated by Beretta (2007). The curve shows how the exergetic efficiency has developed during the last 300 years. The first steam engines at the dawn of the industrial revolution were < 1 % efficient. Today's combined cycle plants reach 55 % efficiency. The ratio between the efficiency over one minus the efficiency is plotted on a logarithmic scale. The linear variation in this ratio with time is typical of many learning processes.

The last point on the curve is, for the time being, the fuel cell. This cell is relevant for a replacement of the combustion engine in cars, to make the transport sector more energy efficient and environmentally friendly. Famous scientists have contributed to the field of thermodynamics, making this curve possible. Lars Onsager, a Nobel prize winner of Norwegian descent, made his discovery of the rules of energy conversion in non-equilibrium thermodynamics in 1931. Improved design of fuel cells may benefit from his theory (Kjelstrup et al. 2010a).

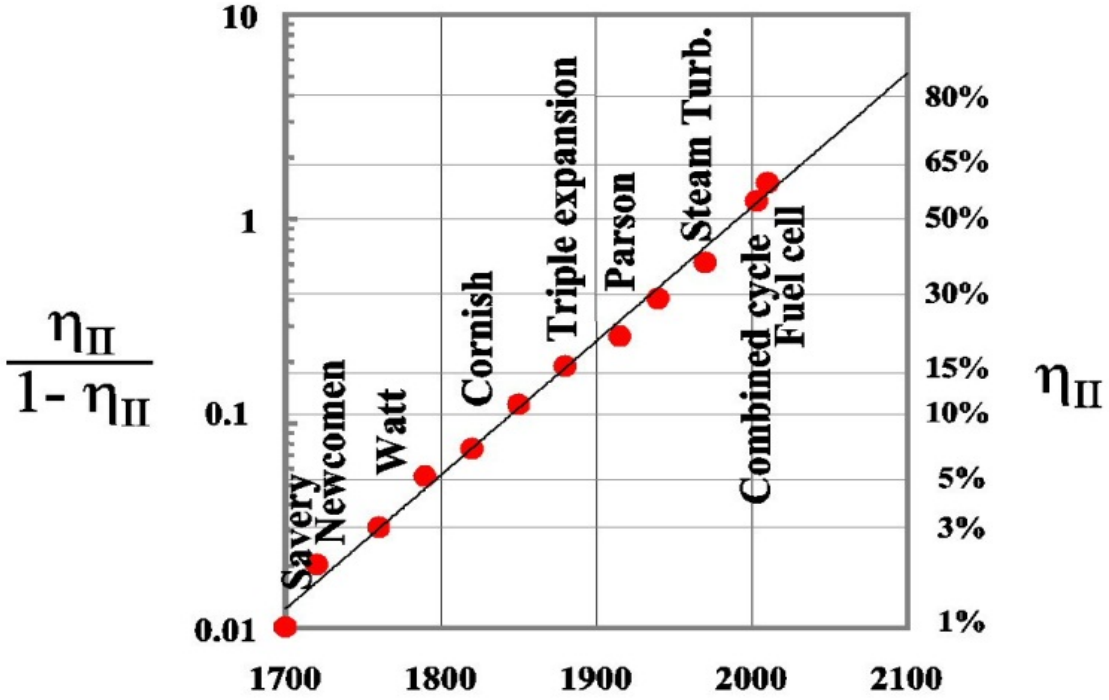


Fig. 2. Development of the exergetic efficiency, ηII, over time according to Beretta (2007).

What is particularly encouraging with the curve is that we have not reached its end point. A limit exists, as there is no process possible without some losses when the process must run in a finite time. Nevertheless, it seems that we can continue to work in this field and learn new important things for quite some time. New power generators can be more dedicated, smaller machines, of electrochemical or optical nature. The field of thermodynamics is now moving to be able to describe smaller and smaller systems on shorter and shorter time-scales. The laws for energy conversion under such conditions are not yet formulated. It is believed that such knowledge can contribute to the variety and specificity that is needed for all the power producing and consuming units that the future will need. The number of PhDs trained at Norwegian universities is not excessive in this context, rather the contrary. In order to foster a development of a multitude of solutions, universities should have an increase in their allotment of PhD positions, to be competed for by the many motivated candidates who want to contribute to this development.

Conclusions and perspectives

We have argued above that the Grassman diagram illustrating exergy consumption in the Norwegian society should be updated, on the national scale, and on smaller scales, for each sector involved. By making maps for the unit or plant level, one can foster a development towards technologies with higher efficiencies, by increased awareness of the single technology and by transfer of knowledge between similar activities and plants.

An exergy map for the Norwegian society can be used to indicate targets for research where a relatively large potential for improvements exists, like for instance the domestic sector. Several definitions of the concept “energy efficiency” exist. We have recommended to use more systematically the exergetic efficiency. Discussions referring to these efficiencies will be more informed, and help politicians and others to make difficult trade-offs. We have given two examples from central Norwegian activities to illustrate possibilities. To foster the development of a multitude of solutions to increase the resource efficiency in the society at large, the universities should be given an increase in PhD positions, for research groups to pursue their ideas with young investigators. A multitude of solutions must be sought.

Acknowledgement The Research Council of Norway and the Norwegian Ferroalloy Producers’ Research Association are thanked for the FUME grant enabling PhD studies of Takla. The Faculty of Natural Science and Technology at NTNU is thanked for the PhD grant for Voldsund. The figures are reprinted with courtesy of Professors Beretta and Ertesvåg.

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Signe Kjelstrup, Mari Voldsund and Marit Takla

NT-faculty MasScenter

The NT- faculty invested in 2012-2013 in two LC ms/ms instruments to be used in a consortium created by the departments of Biotechnology, Chemistry and Biology. The equipment will be used for scientific research and teaching. Main focus of the instrumentation is to provide wide/versatile service to all the different fields included in this consortium. A closer description towards the application of each instrument could be:

LC-MS/MS with high-resolution power (Q-TOF) :
The instrument will be used for study and identification of known and unknown synthesized organic molecules and biological molecules (metabolites, peptides and proteins and other natural products) and for studies of reaction mixtures (mechanistic studies).

LC-MS/MS (Triple quadrupole):
The instrument will be used for quantification and identification of known biological and chemical molecules in complex extracts and mixtures.

One of the main challenges of this consortium is the huge variety of molecules that this MS centre will encounter. Consequently, to this instruments will also be joining them a GC-TOF with Electron Impact ionization.

The sum of all three instruments will grant access to a better multipurpose MS centre and improve its efficiency. Versatility of the lab refers not only to Ionization modes (ESI, APCI, APPI, ASAP and EI), a diversity of separation technologies UPC2 (SCF chromatography) and Capillary Chromatography are also available. Practically all types of chemical compounds can be separated and detected in this lab.

The installation of the instruments is taking place nowadays and will be finished sometime at the end of spring 2013. The MasScenter and the instruments will be later introduced once the lab is operative in a small ceremony /presentation.

Waters
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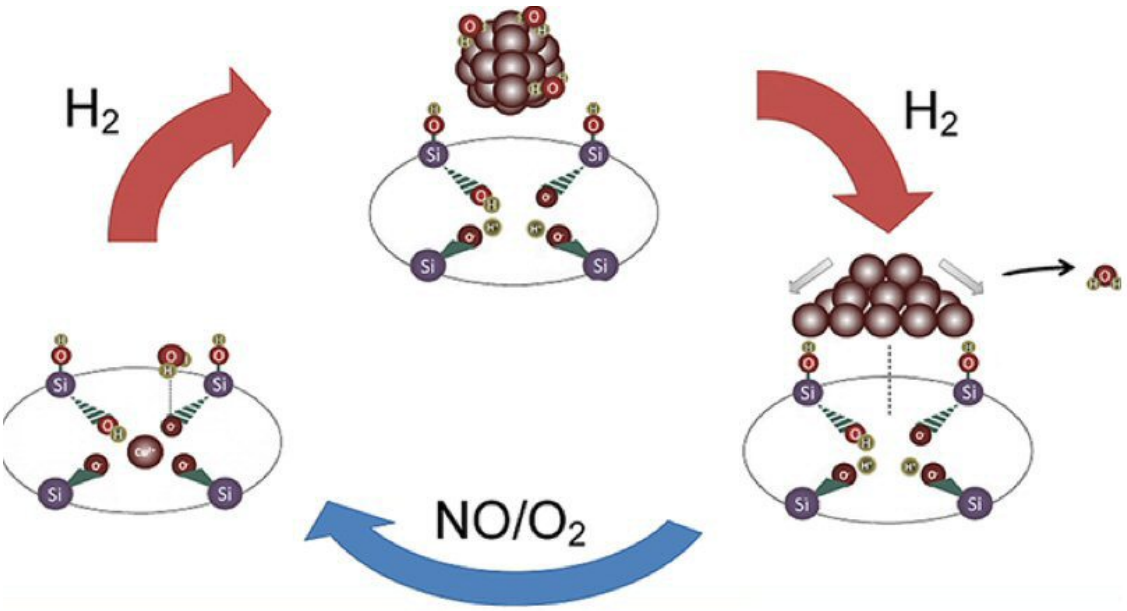
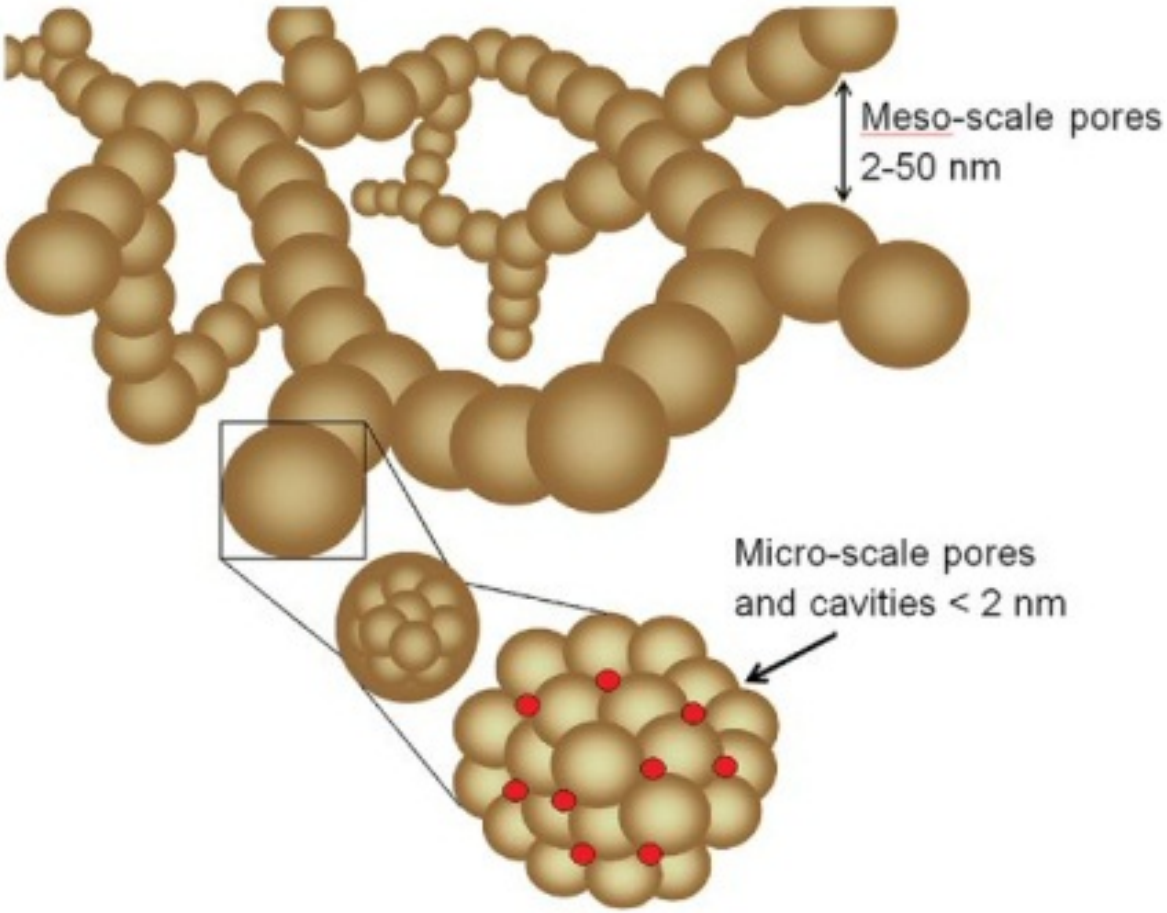
Susana Villa Gonzalez

Materials Science: A Silica Aerogel Copper Catalyst

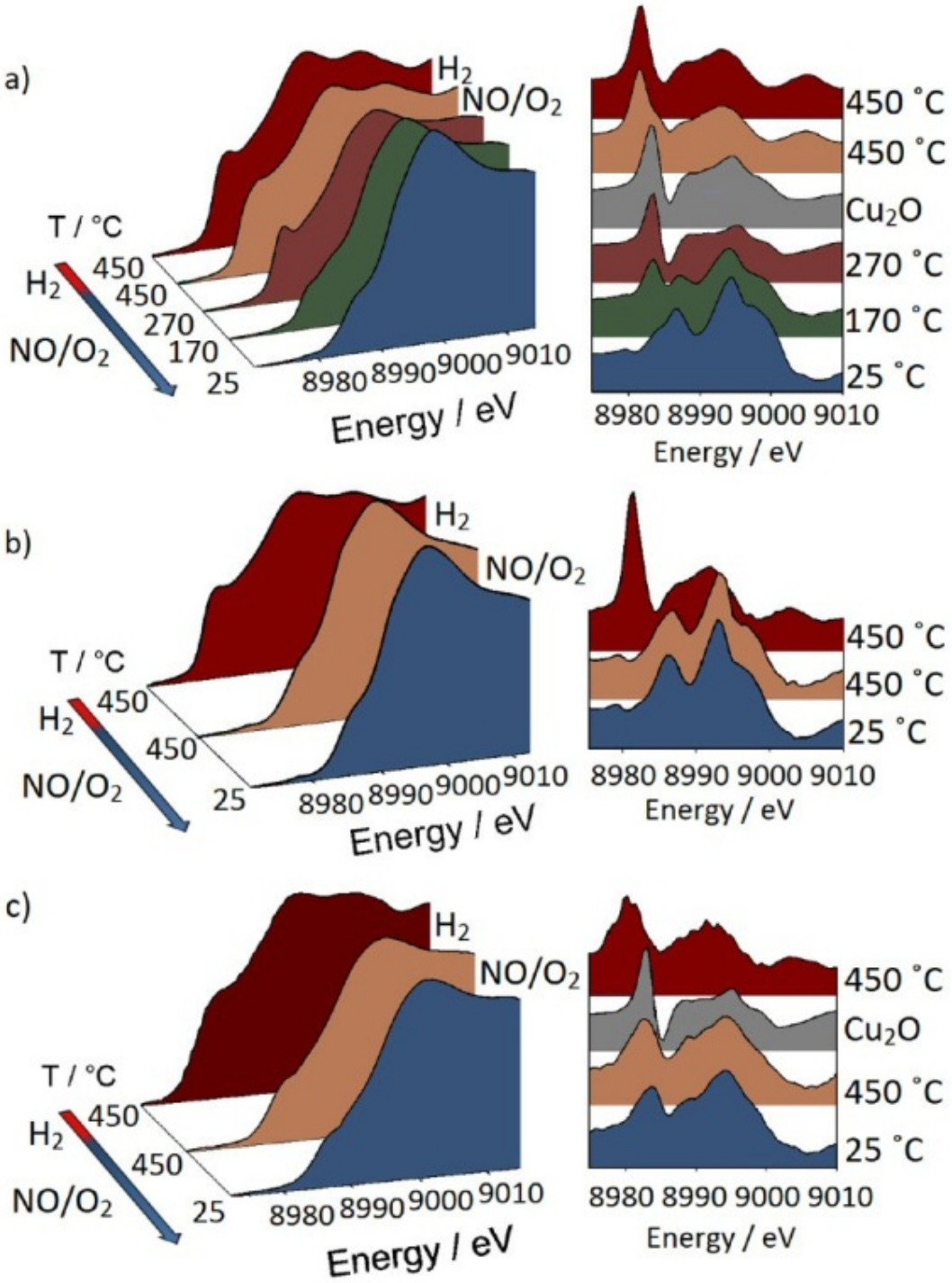
Since 1986 the emphasis on materials science research at the department has been on structural and electronic studies on a variety of chemical systems using the facilities of synchrotrons in the UK (Daresbury) and the USA (National Light Source, Brookhaven and the Advanced Light Source, Berkeley).From 1994 these activities were increasingly centred on the Swiss-Norwegian Beamlines at the European Synchrotron Radiation Facility in Grenoble.
A significant proportion of these investigations have been on crystalline microporous materials which include aluminium phosphates and zeolites. Our interest in these materials is their function as supports for different metals and their compounds which exhibit catalytic properties towards certain processes.These studies have resulted in a number of PhD and MSc theses.
Recently, we have turned to another type of porous system as represented by aerogels. Since there is expertise in this area at the Department of Materials Science we have entered into a collaboration with Mari-Ann Einarsrud.



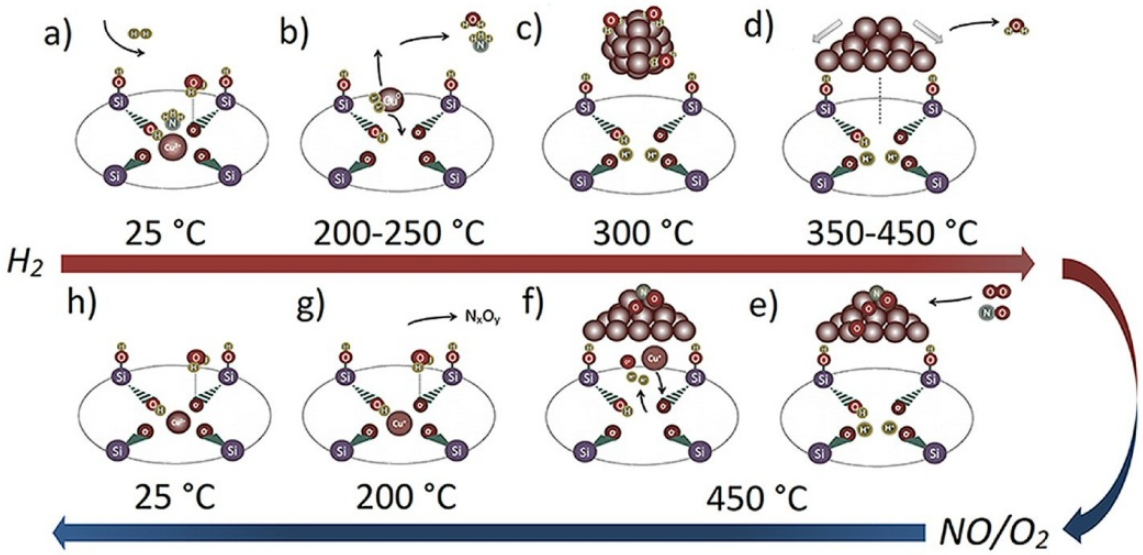
This collaboration is bearing fruit. For example in 2012 the results of a study on the nature of copper in silica aerogels were published [1]. The team consisted of Tina Kristiansen, Karina Mathisen, Mari-Ann Einarsrud, David Nicholson and Jon Støvneng. The latter, who is in the Department of Physics, carried out supporting theoretical calculations. This rather eclectic mix of competences from three departments shows such studies benefit greatly from the pooled expertise.



In the study, copper nanoclusters of around 2 nm were prepared. They are so small that interesting physicochemical effects arise that are very different from the bulk material itself. This means that these ultrasmall particles cannot be compared with normal or bulk copper. The clusters are prepared and supported on a silica aerogel and it is the system as a whole that exhibits special properties that may make it a potential catalyst. Techniques used included synchrotron x-ray absorption and diffuse reflectance infrared Fourier transform spectroscopies, which yield structural and electronic information about the copper clusters and their interactions with the varying local environments provided by gas molecules and the aerogel support. It would seem that the irregular pore sizes and their distributions which characterise the frameworks of aerogels may be the driving force for redispersing copper species over the support. Our measurements show that framework vacancies generate acidic silanol clusters thereby imparting functionality to the support and hence allowing ultrasmall clusters with special properties that influence redox applications such as in catalysis. The figures give a taste of the results described in the paper.



This project was only made possible by SNBL in continuously upgrading instrumentation so as to ensure state-of-the-art facilities



[1] T. Kristiansen, J. E. Støvneng, M. A. Einarsrud, D.G. Nicholson, K. Mathisen,
"There and Back Again: The Unique Nature of Copper in Ambient Pressure Dried-Silica Aerogels." The Journal of Physical Chemistry C 2012 116.(38) 20368

David Nicholson

Towards Effective Nonviral Gene Therapy: Synchrotron Small-Angle X-Ray Scattering Studies on Novel Rigid Gene Delivery Vectors

This project is part of a collaboration between the Department of Chemistry, NTNU and Weill Cornell Medical College, Qatar and the University of Stavanger (UiS); the collaborators being Michael Pungente and Helge Larsen, respectively. These experiments are relevant to a related collaboration with Vassilia Partali´s group because their polyunsaturated cationic lipids are particularly interesting candidates for subsequent studies in 2013 on liposomes and lipoplexes. The synthetic part of this particular collaboration is funded by the Qatar National Research Fund (QNRF) whilst the structural studies (at the European Synchrotron Radiation Facility, ESRF) are funded by NTNU, UiS and the Research Council of Norway.

Introduction

Gene therapy refers to the use of nucleic acids as a potential therapeutic treatment of a variety of diseases, including cancer and inherited disorders such as cystic fibrosis and cardiovascular disease. It involves replacing nonfunctional segments of DNA with functional DNA. Free DNA cannot passively and efficiently cross cellular membranes without the assistance of a delivery agent or vector. These facilitation processes are known as transfection and may be viral or nonviral. Unfortunately, positive results using viruses as the vehicle to carry the therapeutic gene have been overshadowed by pathogenic effects and a few deaths. This has given impetus to studies on nonviral deliveries as an alternative and this is the motivation for this project.

The overall aim of this proposal is use synchrotron small-angle scattering (SAXS) to gain detailed structural information on a series of novel cationic lipid-DNA complexes (lipoplexes) under the influence of a 7.4-5.0 pH-gradient. This information is required to rationalise structure-function relationships. This is necessary for designing more efficient lipid gene delivery vectors that are required for effective gene therapies. Since cationic lipids have a positive charge they complex with the negatively charged DNA thereby forming a lipoplex. The charge means that the lipoplex is able to pass through the cell membrane to release its load of DNA within that cell. It is important to establish the relationship between structure and function of the lipoplex which is where the SAXS method comes in.

The experiments

The facilities of the new BioSAXS beamline (BM29) at the ESRF were used to collect SAXS data on 100 samples of the liposomes* and lipoplexes** prepared from a selection of our lipids. BM29 is a tunable energy beamline (7 - 15 keV) for small angle x-ray scattering (SAXS) measurements on solutions of biological macromolecules. The data allow us to obtain low resolution 3-dimensional structures in a natural environment.

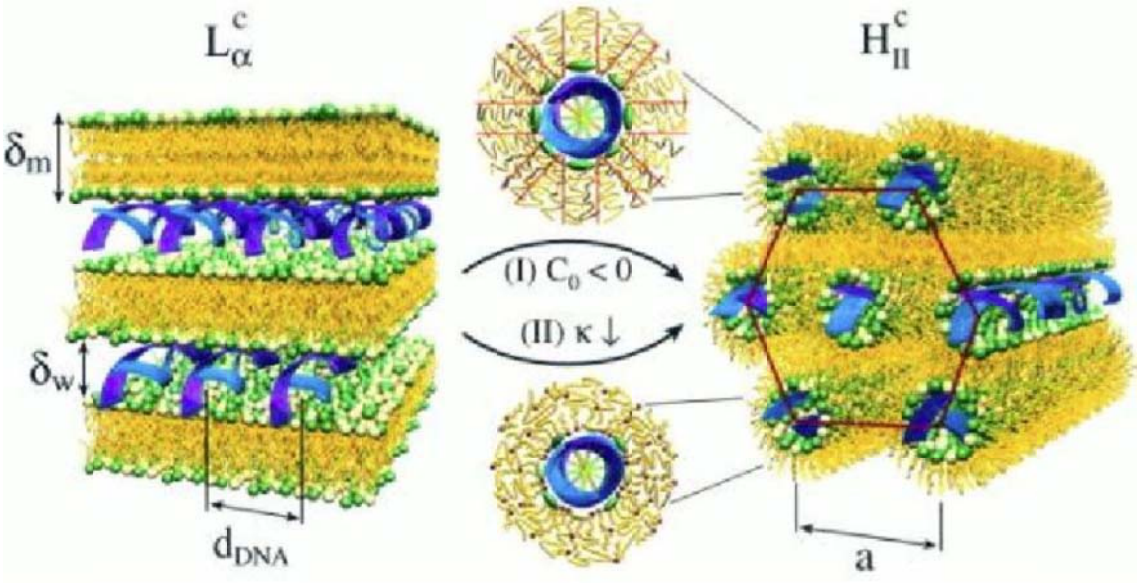


Figure 1 Conceptual depictions of cationic liposome-DNA complex (lipoplexes). DNA helices are blue. The formation of a layered lipoplex (lft) or a hexagonal lipoplex (right depends on the type of cationic lipid used (Koltover, I et al Science, 281, 1998, 78.)

- * liposome - a nanosized spherical sac of phospholipid molecules enclosing a water droplet (a micelle), which can carry drugs or other substances into the tissues.
- ** DNA can be covered with lipids in an organised structure such as a liposome (micelle).

Results

Prior to these measurements, it had been suggested that a pH-induced transformation of a cationic lipid-DNA complex from the lamellar to the inverted hexagonal phase within the endosome is responsible for the release of the DNA cargo [1] We started the experiments partly because of our belief that the lipoplex structural data obtained from SAXS experiments with these novel lipids acquired over a pH-gradient will provide data on the arrangement of the DNA in the lipoplex, the lamella structure and the pH at which the DNA cargo is released as well as possibly some indication as to the structural changes during the process of release. The results demonstrated nicely the diffraction effects that are manifested as discrete peaks at certain angles that arise either from a layered packing arrangement or a hexagonal arrangement (Fig. 2 shows the diffractogram for Vassilia and Richard´s carotenoid lipoplex). Simply put, this means that, in effect, we are seeing powder diffraction from a solution. This is unusual in a bioSAXS experiment and can be appropriately termed small angle x-ray diffraction or (SAXRD). The positions of the diffraction peaks enable us to unequivocally decide which of the two structures applies here, and the corresponding characteristic repetition distance (being δw + δm in the case of Lαc or a in the case of HIIc as given in figure 1).

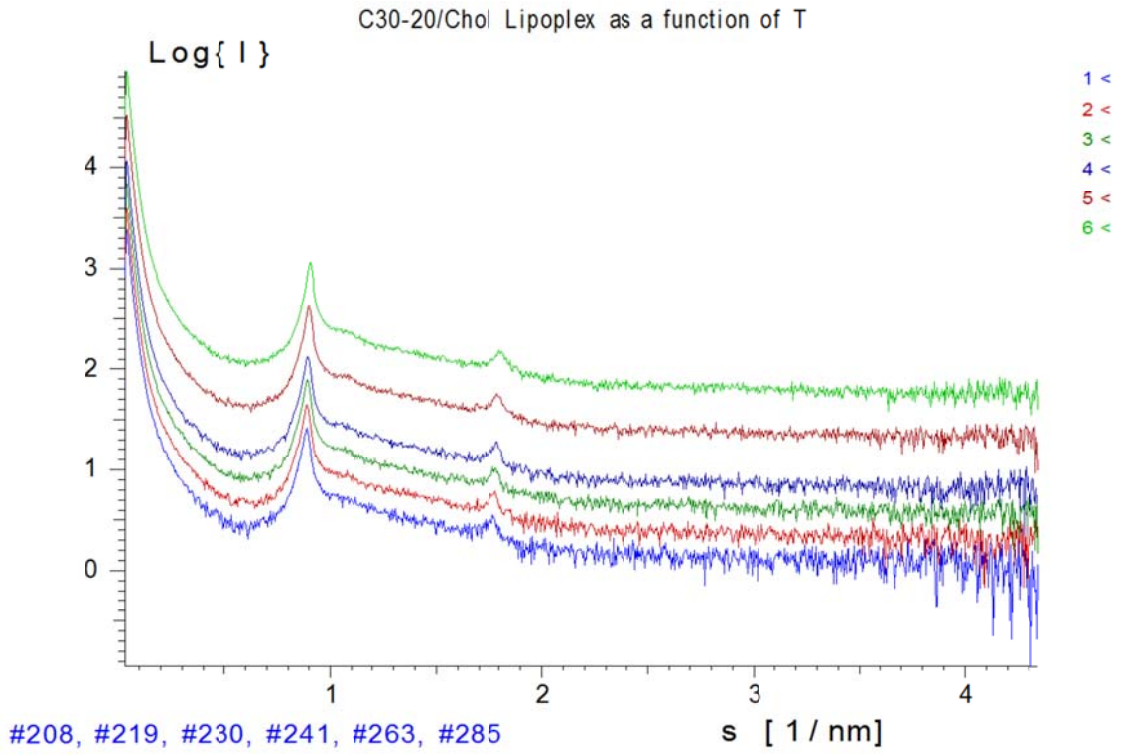


Figure 2. Small angle X-ray diffraction curves for the novel C30-20/Chol Carotenoid lipoplex for different temperatures. The lower (blue) curve shows the result for T = 20˚C, then each new at a temperature increase increment of ΔT = 5˚C. The upper curve is at T = 55˚C. Well defined multilamellar ordering is observed over the whole temperature range. The repetition distance remains quite constant over the temperature interval. A small decrease in δ as the temperature is increased is however noted: δ(T = 20˚C)= 71.1 Å to δ(T = 55˚C)= 69.7 Å. The curves are shifted along the ordinate axis for clarity.

The way forward from here is to correlate with in vitro transfection efficiency data in the hope that we can reveal lipid structure-function relationships. Ultimately, we wish to identify a refined and more effective gene delivery vector.

References:

1.Bell, P.C.; Bergsma, M.; Dolbnya, I.P.; Bras, W.; Stuart, M.C.A.; Rowan, A.E.; Feiters, M.C.; Engberts, J.B.F.N. J. Am. Chem. Soc. 2003, 125, 1551.

David G. Nicholson

Applying Synchrotron Radiation to Studies in Cultural Heritage

The main thrust of the Department of Chemistry´s research activities at the Swiss-Norwegian Beamlines (SNBL) at the European Synchrotron Radiation Facility in Grenoble, France has mainly been confined to materials chemistry.

However, in recent years there is an increasing awareness that synchrotron radiation can also be applied to problems related to Cultural Heritage and that studies here resonate with the general public. This is recognised by the SNBL and the ESRF both of which have made room for Cultural Heritage proposals.

A high profile example from the ESRF is a study on some of van Gogh´s paintings in which bright yellow pigments are becoming dull brown when exposed to UV and sunlight. Understanding the slow chemical changes occurring over the years is a necessary prerequisite to any attempt at preservation or conservation and this is where results from synchrotron radiation investigations are important. These experiments give information on structural and electronic changes and their causes.

The results of such studies have entered the public domain through newspapers and broadcasters, for example the BBC[1][2]. Obviously, van Gogh´s works are very much in the public eye and the realisation that the original bright yellow colours used by the pointer in, for example, his sunflowers are being discoloured has cause considerable consternation amongst collectors, museums and the art-loving general public.

The synchrotron experiments examined the properties of a yellow pigment but other investigations are much broader; we report below, as a case study, the first Chemistry Cultural Heritage experiments at the. The experiments, which were carried out in My 2012, are part of Kidane Fanta Gebremariam PhD project on characterising pigments in murals from medieval Ethiopian Churces..Kidane is a member of Lise Kvittingen´s Cultural Heritage group at the Department of Chemistry Research is ongoing and follow-up experiments will be performed in 2013, also at SNBL and possibly at a complementary ESRF beamline.

This case study is a good example of the practical use of synchrotron radiation in studying aspects of Chemistry in Cultural Heritage in general and at the SNBL in particular.

[1] BBC report showing examples of pigment degradations. http://www.bbc.co.uk/news/science-environment-19597399

[2] Another BBC report describing another use of synchrotron radiation in revealing hidden secrets in van Gogh´s work.
http://news.bbc.co.uk/2/hi/europe/7535574.stm

David G. Nicholson

Characterisation of pigments in murals from two medieval period Ethiopian Churches using Synchrotron X-Ray Diffraction and Micro-Raman Spectroscopy

Introduction

The preservation and conservation of cultural heritage has increasingly been given more attention all over the world [1]. As a result of this, there is a corresponding increase in demand for fast, robust, reliable, in situ and non-destructive analytical techniques for studying artistic and archaeological objects. The technical examination of painting materials and the choice of technique is essential for conservational interventions besides a supplementary role in art historical investigations. Results from such investigations can be useful for various purposes such as dating, authentication, provenance studies, insight into early trade links and material technology [2]. It also paves the way for comparative studies of paintings produced in different traditions and regions.

Despite the large number of Ethiopian works of art existing in the forms of murals, icons and illuminated manuscripts produced by an old traditional style of painting, studies from the chemical perspective are scant. The wall paintings being investigated in this research belong to a 12th century and 13th century churches in Ethiopia: Yemrehana Krestos and Genete Mariam, respectively. These churches, which contain relatively well dated wall paintings, are in a poor state of conservation [3]. They are located close to Lalibela, a UNESCO cultural heritage site of eleven rock-hewn churches.

The main objective of the experiment was to identify the different mineralogical phases of the painting materials in the painting samples using high resolution x-ray diffraction (XRD) and micro-Raman spectroscopy. Prior investigations based on optical microscopy and scanning electron microscopy have proved useful in identifying some of the materials contained in the painting and preparatory layers. However, the elemental information needs to be complemented by molecular and crystal structural techniques. The later techniques can be used to reliably establish the identity of the pigments, plasters, extenders used and the degradation products due to ageing and environmental impact.

Scientific background

The non-destructive investigations are the most preferred ones as keeping the integrity of the cultural heritage is given the utmost priority all the time from the ethical perspective. Analysis of pigments has been carried out in situ on the wall paintings of the two churches using a portable x-ray fluorescence (XRF) analyser. Following the survey of the elemental composition of the different colours in selected paintings in the two churches, micro-samples were taken to study stratigraphy of the paintings, morphology of the painting materials, the composition of pigments and plaster layers. Embedded in acrylate resin and polished, the resulting cross-sectioned samples were subjected to examinations by Polarised Light Microscopy (PLM), Fluorescence Microscopy and Scanning Electron Microscopy-Energy Dispersive Spectroscopy (SEM-EDS).

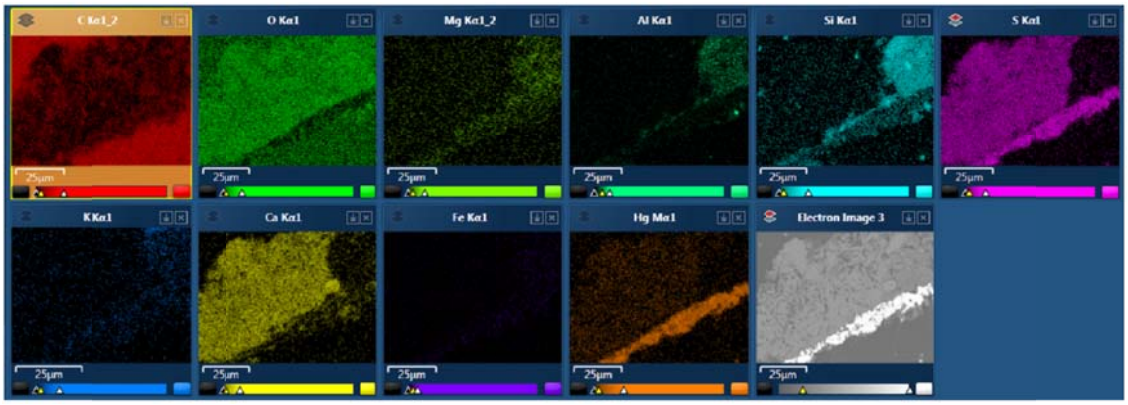


Fig 1. EDS mapping of the elemental composition of a red paint sample from Yemrehane Krestos Church. The gypsum preparatory layer and the cinnabar rich painting layer are clearly visible. The aluminosilicate indicated at the surface of the painting is due to dust accumulated through years.

The unambiguous identification of painting materials needed not only elemental analysis but also molecular, mineralogical and structural information which can be acquired from XRD and Raman Spectroscopy. Considering the multilayer painting structure and the complex mixtures of compounds in micro-samples, high spatial resolution coupled with good sensitivity is highly demanded. High-resolution X-ray powder diffraction based on intense, low noise, monochromatic and highly collimated synchrotron radiation as well as Raman spectroscopy can serve this purpose [4-6]. High spatial resolution is essential for phase targeting that can allow the identification of minor components belonging to the original painting materials, weathering products, surface contaminants, and later conservation interventions.

The main objective of the experiment was to use high resolution XRD and Raman spectroscopy for the identification of molecular components and crystalline phases of the pigments and plasters in the painting samples. Some test experiments have already been run at Swiss-Norwegian Beam Lines (SNBL) of the European Synchrotron Radiation Facility (ESRF) in Grenoble, on few cross-section samples using synchrotron X-ray powder diffraction (SR-XRD) and micro-Raman techniques providing promising results.

Fig 2. Raman experiment using Renishaw inVia Raman microscope at SNBL.

Experimental technique

High Resolution Powder Diffraction and Micro Raman Spectroscopy

Synchrotron XRD and Raman measurements were carried out on the different painting samples collected from the wall paintings of the two churches. The crystalline phases were characterised by high-resolution powder diffraction (HRPD) measurements at station BM01B. Similar setup used at the station for pigment analysis earlier was employed [7]. The system consists of a two-circle diffractometer with six lined-up detectors. The diffractometer is equipped with 6 counting chains (i.e., 6 complete patterns are collected simultaneously). A Si-111 analyser crystal is mounted in front of each detector (NaI scintillation counter), resulting in an intrinsic resolution (FWHM) of approx. 0.01 deg at a wavelength of 1 A. The wavelength used for the experiment was 0.5035046 Angstroms. The very small samples used in this technique are non-embedded micro samples placed in a capillary tube.

Raman measurements were made with a Renishaw inVia Raman microscope system. The power of the laser beam can be adjusted with a set of filters to allow measurements with appropriate fraction of the initial radiation power. Most of the measurements were carried out in the duration of 60s, with 1-10 accumulations. A laser with a wavelength of 785 nm will be used as an excitation source.

Fig 3. High resolution XRD experiments being conducted on some of the painting samples at section BM01B of the SNBL.

Prior SR-XRD measurements

XRD data from cross-section samples were collected using the MAR345 image plate detector at SNBL, station BM01A. The painting samples were embedded and polished in fast curing methyl methacrylate-based resin under blue light. The phase analysis was conducted using X'Pert HighScore Plus program and the PDF-4 database.

The background originating from the embedding medium was subtracted. The wavelength used was 0.6973Å and the exposure per frame, 30s. The sample-to-detector distance was set at 250mm. The beam size was measured 300microns x 300microns. All data were collected at room temperature.

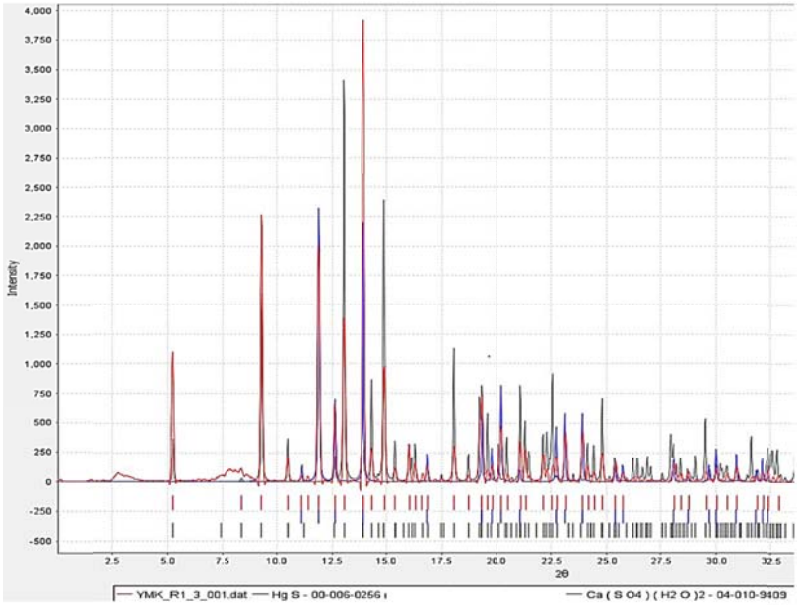


Fig 4. Confirmation of the pigments identified using SEM-EDS using XRD measurement at BM01A station of SNBL. Metacinnabar, a black mercuric sulfide and polymorphous with cinnabar was identified. Besides gypsum (CaSO4.2H2O), the anhydrous counterpart, anhydrite (CaSO4), was also identified in the preparatory layer.

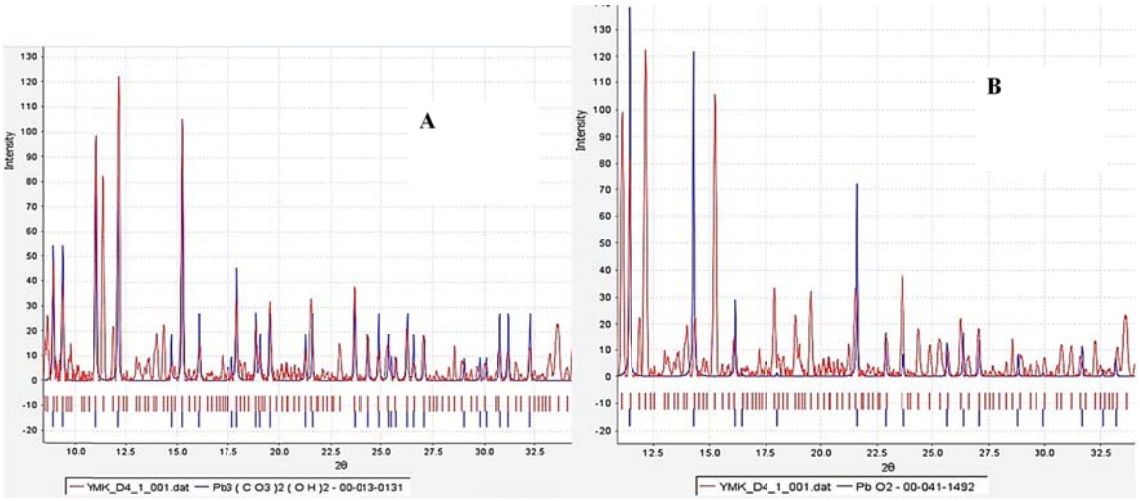


Fig 5. Diffraction patters that helped to identify lead white in a micro painting sample (A) and one of the degradation products of lead white - plattnerite (PbO2) – a dark compound (B). The sample appears dark and lead was identified from SEM point\mapping analyses and Back-scattered Electron (BSE) images. The measurement was done at SNBL, station BM01A.

References

1. Z. Szõkefalvi-Nagy, A. Kocsonya, I. Demeter and I. Kovács Nuclear Instruments and Methods B226 (2004), 53-59.
2. R.J.H. Clark, C. R. Chimie 5 (2002) 7–20.
3. D. W. Phillipson, Ancient Churches of Ethiopia, New Haven: Yale University Press, 2009.
4. N. Salvado, S. Buti, M.J. Tobin, E. Pantos, J.N.W. Prag, T. Pradell, Anal. Chem. 77 (2005) 3444.
5. 5 N. Salvado, T. Pradell, E. Pantos, M.Z. Papiz, J. Molera, M. Seco, M. Vendrell-Saz, J. Synchrotron Radiat. 9 (2002) 215.
6. D. Creagh, in: D. Bradley, D. Creagh (Eds.), Physical Techniques in the Study of Art, Archaeology and Cultural Heritage, vol. 2, Elsevier, 2007, p. 1.
7. N. Salvado, S. Buti, J. Nicholson, H. Emerich, A. Labrador and T. Pradell, Talanta 79 (2009), 419–428.

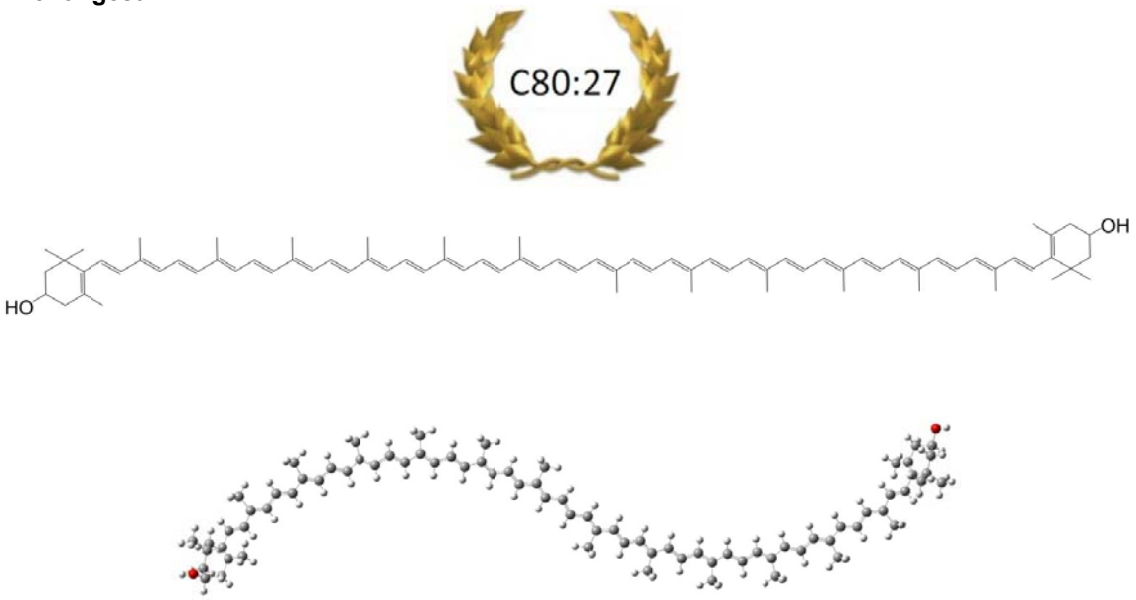
Kidane Fanta Gebremariam

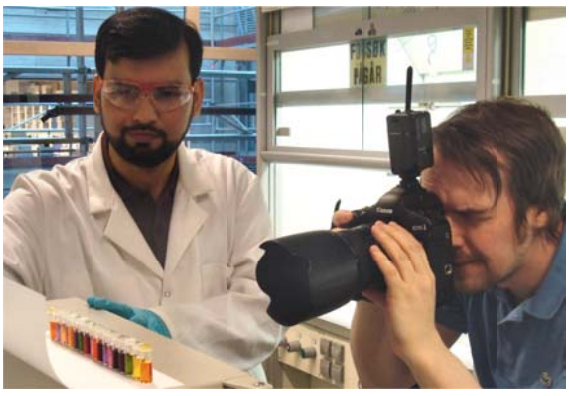
The longest polyene

Length is a sensitive matter in the extension of conjugated polyenes. Common experience tells: too long = not enduring. *Mohammad Zeeshan* has modified the classical Wittig reaction allowing polyene elongating to 27 double bonds without substantial detriment for stability. The 60 years old unchallenged record of 19 double bonds has now been beaten by elongation with 8 additional C=C units. Molecular modeling showed the typical bended structure for polyenes

Richard Sliwka, Vassilia Partali

The longest





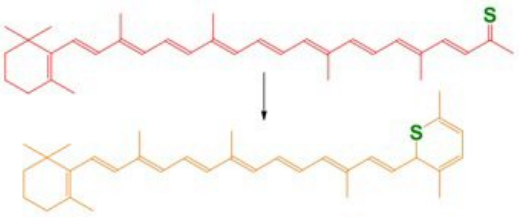
Double bonds are chromophores and 27 in conjugation appear violet. The flamboyant microwave synthesis (described in Org. Lett. 2012, 14, 5496) has not gone unnoticed and a professional photographer took several pictures of Zeeshan's colorful product palette.

The longest polyene is the 7th from left, the other colors represent polyenes of different lengths.

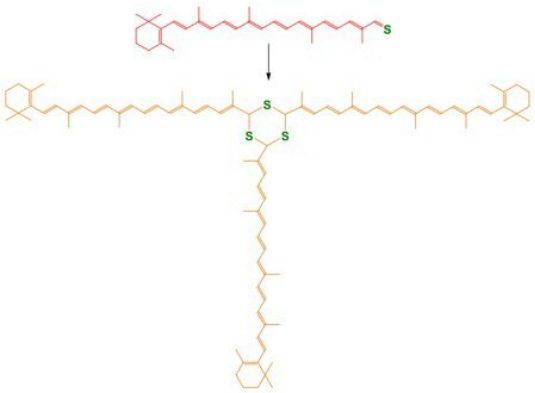
Sulphur is different

Carbonylcompounds such as aldehydes and ketones are generally stable and their odor is rather pleasant. Thiocarbonylcompounds [thioaldehydes (thianes) and thioketones (thiones)] are unstable and their odor is often distasteful.
Polyene monothiones can be stable and their fragrance is quite delicate. However, polyene dithiones were unstable and *Gina Sandru* found that there is no time for smelling. She could just hurry to record a uv-vis spectrum. It confirmed what she has seen: the orange carotenones get a blue hue, the thiocarbonyl function shifts the absorption to longer wavelengths.

Other polyenethiones are very reactive and instead of giving a shift to longer wavelength, they absorbed at shorter absorption maximum. Gina saw the orange solution becoming yellow. With the help of *Nebojsa Simic's* many NMR spectra and *Susanna Gonzales'* MS spectra it was found that a surprising thiopyran cyclization occurred (*Tetrahedron Lett.* **2012**, *53, 6822*).



Polyene thials are very reactive and trimerize to dendrimer like compounds.



The sulphur compounds will be used for self-assembling on Au surfaces and Au nanoparticles.

PhD candidate Gina Sandru together with former master student Marius Myreng Haugland, now PhD candidate in Oxford.

Richard Sliwka, Vassilia Partali

"Nonviral Delivery of Therapeutics" A New International, Multidisciplinary Collaborative Research Group

There is considerable activity in searching for effective gene therapies that involve transferring nucleic acids as a pharmaceutical into cells so as to beneficially modify those genes that are responsible for a wide range of diseases. Unfortunately, positive results using viruses to carry the therapeutic gene have been overshadowed by pathogenic effects and actual deaths. This has given impetus to studies on nonviral deliveries as an alternative.

One type of transfer vehicle that may be promising in this regard is the class of compounds known as saturated cationic lipids. Chemists at the Department of Chemistry have recently synthesised polyunsaturated cationic lipids, which, being coloured, do not need a fluorescence tag for biological tracking. These compounds have been highly appreciated by biochemists at the Weill-Cornell Medical College in Doha and this has lead the Qatar National Research Foundation to support this collaboration with a generous grant.

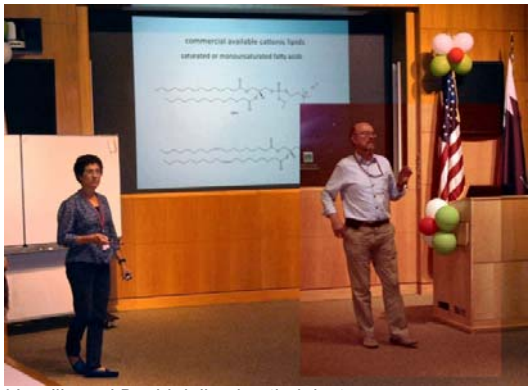
The project has been productive and we have arrived at the stage where it is necessary to establish structure – function relationships in order to be able to move forward in the right direction. Accordingly, the Synchrotron Group at the Department of Chemistry, in association with the University of Stavanger, is collaborating in this area.

Funding for the NTNU- Qatar collaborative project expires 31.08.2013 and to round off this effort a workshop was organised in Doha, Qatar in November 2012.The workshop had an additional role, to set out possible routes for further collaborations that spring out of the positive results of the current project. In order to achieve this, well-known capacities in biomedical areas were invited to take part.

During the first part of the workshop, Vassilia Partali reported progress in the context of gene therapy on studies of cationic lipids based on highly unsaturated conjugated fatty acids. David Nicholson introduced methods used in studying the structures of lipid-DNA complexes such as small angle scattering of synchrotron-generated x-rays. Richard Sliwka initiated the discussion on the way forward by describing a system of selena cationic lipids self-assembled on gold nanoparticles and that this system could be a key part of the nonviral gene therapeutic project under planning.

The plenary discussions centered around using the gold-lipid system in therapies for several diseases in particular neuromuscular disease and lung cancer and the importance of structure – function relationships.

The outcome of the workshop is the agreement to form a new collaborative group that will include amongst others, NTNU (organic chemistry and the synchrotron group), Weill Cornell Medical College, University of Stavanger, Royal Holloway University of London, Paris Descartes University and Universidad National Autonoma de México. It is hoped to start and define this collaborative activity by the summer of 2013.



Vassilia and David delivering their lectures

Round table meeting in Doha

Vassilia Partali, David G. Nicholson, Richard Sliwka

قطـر

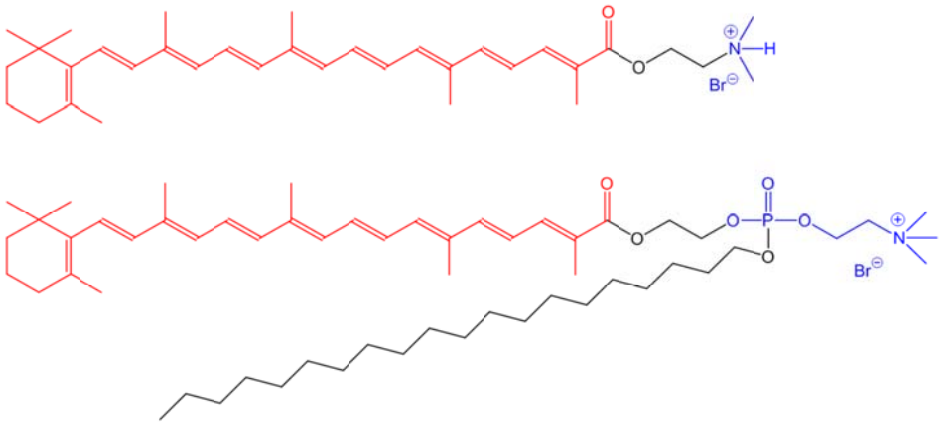
Highly unsaturated cationic lipids as gene carriers

Medical treatment by pharmaceuticals given to patients with exogenous diseases is well known. However, the medication of endogenous, genetically inherited illnesses such as cancer, muscular dystrophy, Alzheimer, Huntington, thalassemia, hemophilia, etc. is in its infancy. Gene therapy works by replacing either the disease-causing genes with good ones or by suppressing the influence of the abnormal genes. Gene therapy depends on specific biological, chemical or physical procedures, which transport various nucleic acids (NA) into the cell. Promising carriers are cationic lipids. These molecules can transport a high NA payload and are not pathogenic. We have replaced the saturated fatty acids in these lipids with highly unsaturated conjugated fatty acids, e.g. retinoic acid and food color E160f. In cooperation with a group at Weill-Cornell Medical College Doha and the Royal Holloway University London, supported by a grant from the Qatar Science Fond, *Christer Øpstad's* lipids were applied for in vitro tests. The most unsaturated compounds showed encouraging results for siRNA delivery into cervix cancer cells and into human skeletal muscle primary cells. Gene transfer to the latter cells could help to cure Duchenne muscular dystrophy (*Molecules* 2012, *17*, 1138; *Molecule*s 2012, *17*, 3484; *Patent application* US201261721975).

At work in Weill-Cornell (Doha)

Preparation for oriental research in Doha. SJA carried out with regard to UV radiation and sharks.

Richard Sliwka, Vassilia Partali



Secondary organic aerosols from biological origin

A collaboration between NTNU and IRC Lyon

Isoprene from natural sources

Isoprene, a compound emitted by vegetation, could be a major contributor to secondary organic aerosols (SOA) in the atmosphere. Isoprene is the structural unit contained in several natural products (isoprenoids), such as mono-, sesqui, di- and triterpenoids, which are common constituents of many varieties of trees and plants.

Isoprene oxidation products in atmosphere

The main evidence for this contribution was the 2-methylbutane-1,2,3,4-tetraols (1), or 2-C-methyl erythritol and 2-C-methyl threitol (sugar nomenclature) (Scheme 1) present in ambient aerosols (measured by GC-MS) in the atmosphere above the Amazonian rain forest. (Claeys et al., 2004) It was postulated that these compounds were formed by photooxidation of isoprene (2-methyl-1,3-butadiene) in the atmosphere. Fig 1.

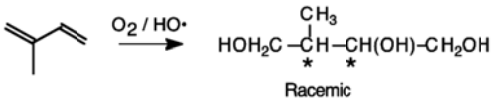


Fig. 1

Convolvolus arvensis

Although it was claimed by the authors of the Science article that the tetraols were not previously known, 2-C-methyl-D-erythritol (2R,3R-1) was isolated from a plant source in 1976. (Anthonsen, et. al., 1976) Fig. 2.

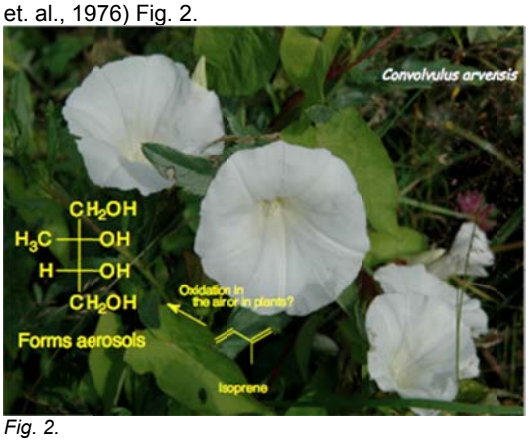
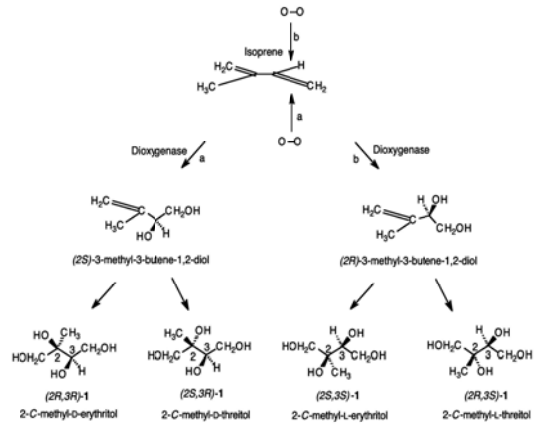


Fig. 2.

The structure has been fully elucidated, also with respect to stereochemistry. (Anthonsen, et. al., 1980) The tetraols 1 have two stereogenic centers and thus may exist as four stereoisomers, see predicted biosynthesis in Scheme 1.



Scheme 1

All four isomers have been synthesised by chemo-enzymatic methods (Moen, et al., 2007)

Stereochemistry

There are two enantiomeric pairs (mirror images), 2S,3R-1 and 2R,3S-1 and 2R,3R-1 and 2S,3S-1. The isomers that are not mirror images, are diastereomers. Diastereomers are different compounds, with different melting points, boiling points etc. Enantiomers are different only when they interact with objects which also are chiral, such as when our “enatiomeric” hands interact with an “enantiomeric” pair of gloves.

Photooxidation vs. biosynthesis

Synthesis of pure enantiomers is difficult. In order to produce enantiopure products, a chiral principle must be involved. In Nature, enzymes are the chiral catalysts. If isoprene is oxidised to tetraols catalysed by enzymes, there will be a non-equal distribution of the stereoisomeric products. An atmospheric photooxidation, with no chiral catalyst, will give an equal distribution of enantiomeric products. However, oxidation products which are diastereomers, such as erythro/threo, will not occur in equal amounts because transition states for their formation have different energy. In the absence of a chiral principle there should be formed equal amounts of 2S,3R-1 and 2R,3S-1 and also of 2R,3R-1 and 2S,3S-1.

Biological origin of 1 in Aspvreten
The four stereoisomers of these tetraols were analysed in aerosols from Aspvreten, Sweden. 2-C-methyl-D-erythritol (2R,3R-1) was found in excess over its enantiomer (2S,3S-1) in the spring/summer, by up to 29 % in July. (Noziére et al., 2011) Fig 3.

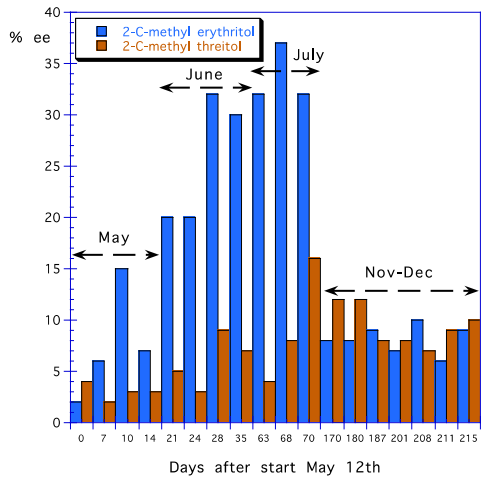


Fig. 3

Chiral chromatography
The collected aerosol samples were analysed by chiral GC with internal standards. This clearly indicated some biological origins for this enantiomer, consistent with its well-documented production by plants and other living organisms.

Aerosols affect climate
Atmospheric aerosols affect the climate directly, through the scattering and absorbtion of sunlight, and indirectly, by functioning as seeds for cloud formation.

Further investigation of aerosols
In order to investigate if other isoprene oxidation products are present in atmospheric aerosols, collection of air samples from different areas will be performed. Synthesis of standards, such as tetraols, terpenoids, carbohydrates, peptides etc and herbicides and insecticides will be performed and used for quantitative investigations of organic compounds in atmospheric aerosols.

Master student Karin Glansberg is at the moment testing different substrates and enzyme preparations for optimising the synthesis of enantiopure 2-C-methyl-D-erythritol (2R,3R-1) and its isomers.

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Elisabeth Jacobsen, Thorleif Anthonsen

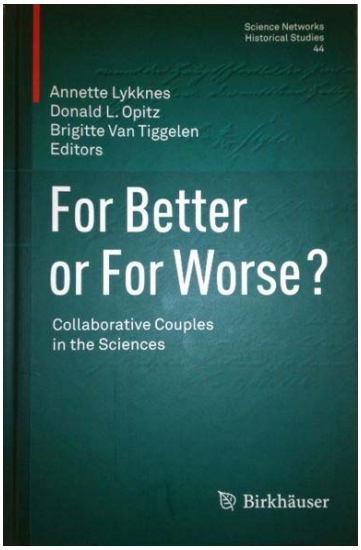
Cultural Heritage: Highlights

A group of academic staff* with interests in cultural heritage established a thematic research and teaching group to advance activities in this increasingly active field. Chemical Education is included amongst the group´s interests.

The following highlights are selected for 2012.

For Better for Worse? – Collaborative Couples in the Sciences

We know the story about Antoine Lavoisier who, sadly, was guillotined during the French Revolution, but there is not the same awareness about his wife´s role as his amanuensis. In the eighteenth century weight was not given to collaboration between couples in the same way as in the nineteenth and twentieth centuries. It is this period which is researched in the book [1] with the same title as the above heading. Annette Lykknes is one of the editors and authors. The theme of the book is to examine the nature of scientific collaborations between couples in the nineteenth and twentieth centuries. Whilst the fates of the protagonists covered by the book are not fully as dramatic as Lavoisier´s there are nevertheless some good stories.



For anyone interested in the shifting mechanisms of human interactions it is fascinating to see how personal and professional dynamics can either foster or inhibit scientific activities. Indeed, the subject is very relevant for NTNU today; for example, on our own doorstep we have the husband and wife team which leads the Kavli Institute and the Centre for the Biology of Memory.

Stories behind a number of fruitful collaborations are told; Annette´s contribution being a study on the research carried out by the German chemist Walter Noddack and his wife Ida Noddack-Tacke with a poignant ending for Walter. For those who have forgotten, Walter and his wife together with Otto Berg reported the discovery in 1925 of rhenium (element 75). Rhenium, which has nine valence states (and is chemically similar to the radioactive technetium) was the last stable element to be discovered. Incidentally, this element has entered into main stream chemistry and figures in a synchrotron study carried out on a catalyst at the department. Ida was the first woman to study chemistry at the Technical University of Berlin and she was nominated three times for the Nobel Prize in Chemistry.

Chemistry and Cultural Heritage: A practical reconstruction from the Keuterbuch, of Adam Lonicer 1559

NTNU has joined forces with the National Library of Norway and Sant'Anna School of Advanced Studies, Pisa, Italy to fund a multidisciplinary digital library, MUBIL. The project aims to develop a virtual learning space and uses 3D technology to allow visitor interaction at different levels (see http://www.ntnu.no/ub/omubit/bibliotekene/gunnerus/mubil).

The Department of Chemistry through Lise Kvittingen has been invited to participate in the project involving the digitalising of Adam Lonicer´s book of 1559, Keuterbuch an example of which is in the possession of the Gunnerus Library, NTNU.

Using text and figures depicted in the Keuterbuch, Fredrik Motland Kirkemo, a MSc student in the Department of Chemistry, has reconstructed a full scale distillation furnace(Figure). This is installed adjacent to Suhm House on the Gløshaugen campus.

The experience gleaned from this work is integrated into a contextual framework that provides a narrative of interest both to academia and to a broader public.

The project is part of the Department of Chemistry´s activities in Chemistry and Cultural Heritage, a field which has been largely ignored in Norway despite there being many artifacts that deserve to be studied from the viewpoint of conservation, preservation and not least dissemination.

Figure 1: To the left one page from Lonicer's Kreuterbuch. To the right a reconstructed and working distillation furnace in Norway in November, as described in Lonicer's Kreuterbuch. Some of its paraphernalia are visible through the vapour such as specially shaped bricks, "Moor's head" of reticulum, gasket of intestines, curcurbit and helmet, as well as the "starke wasser" nicely distilling from the beak.

Writing the History of High- Performance Liquid Chromatography

The Chemical Heritage Foundation in Philidelphia is a library, museum, and archive which was founded in 1982. The Foundation is a collections-based nonprofit organisation that preserves the history and heritage of chemistry, chemical engineering, and related sciences and technologies. Studies are undertaken on the pioneering and landmark instruments used in scientific research. The collections illuminate the role of chemistry in shaping society. A major commitment is to build a vibrant, international community of scholars. One of these scholars is our own Apostolos Gerontas. Who was awarded the Doan Fellowship for four months in 2012 in order to carry out archival research on High- Performance Liquid Chromatograph or HPLC. This type of instrument is an important part of the instrumentation of organic laboratories.

Apostolos has been specially invited to present results of this work in a kick-off lecture to the Symposium for Collaborative Activities at Large Experimental Systems (SCALES) to be held near Perpignon, France in March 2013.

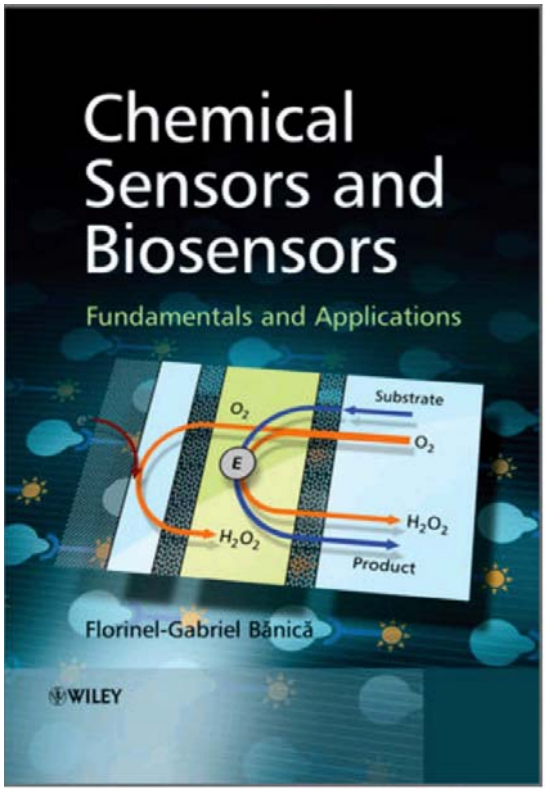
Figure An application of HLPC is to analyse alkaloid content in poppies

Chemical Education: Chemical Sensors and Biosensors

The heading refers to the 531page textbook written by Florin Banica and published by Wiley. The group is pleased to acknowledge this work as a highlighting our contributions to chemical education. Also available are PowerPoint slides for teaching purposes.

The book starts out by referring to the Canadian philosopher Marshall McLuhan who had controversial (at the time) views on media which he regarded to be extensions of some functions of the body. (McLuhan predicted the World Wide Web nearly thirty years before it arrived.) The relevance to McLuhan is the point that chemical and biochemical sensors can be considered to be extensions of those organs of chemical perception, the nose and tongue. The book reflects the fact that chemical sensors play increasingly active roles in society so much so that they are perhaps taken much for granted by the general public. Examples include chemical sensors in the food industry, healthcare, environment and agriculture. The book is impressively comprehensive in its scope and is intended to be not only a teaching aid for courses dealing with a variety of sensors but also for those scientists and engineers who need to become acquainted with the field.

Apostolos has also contributed a chapter on this subject to Zur Geschichte von Forschungstechnologien published by GNT-Verlag.



** Florinel Banica, Lise Kvittingen, Annette Lykknes, David Nicholson, Kidana Fanta Gebramariam, Apostolos Gerontas and Gebrekidan Mebrahthu Tesfamariam.*

David G. Nicholson

X-ray attenuation factors in fluorescence intensity emission - effects of finite sample size

This is a project that results from my role as Visiting Professor at the University of Stavanger and is one of several collaborative projects in the Department of Mathematics and Natural Science. My collaborators in Stavanger are Helge B. Larsen and Gunnar Thorkildsen. This collaboration has resulted in a publication (which was selected by the journal as a highlight for 2012). [1]

X-ray absorption spectroscopy (XAS) has advanced significantly as a structural technique since being introduced in 1986 to AVH (Rosenborg) as a research tool. Over the years the method has progressed from being initially regarded with some justifiable skepticism, to its current status as an invaluable method for studying various chemical systems, particularly those within the areas of catalysis and materials science.

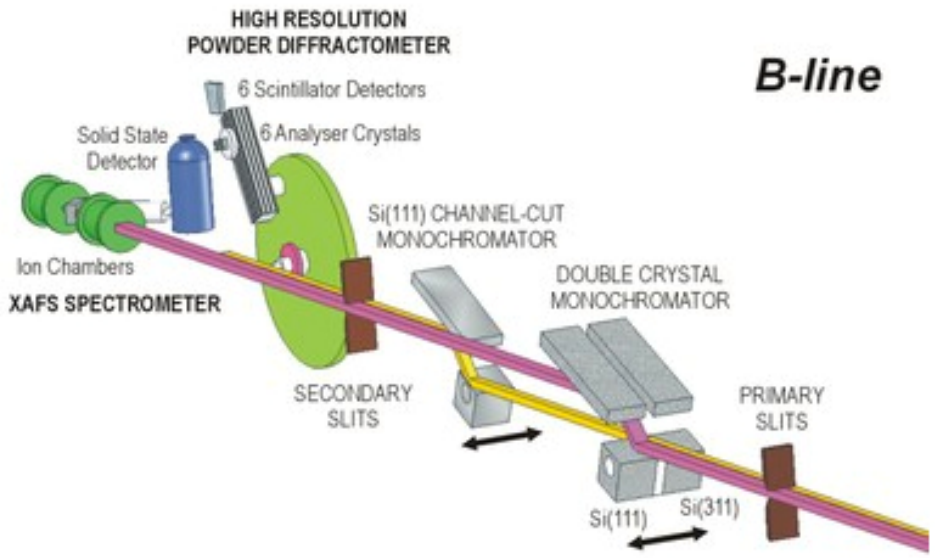


Figure. Schematic layout of the High Resolution Diffractometer and XAFS Spectrometer at the Swiss-Norwegian Beamlines at the European Synchrotron Radiation Facility, Grenoble.

This change is due to improved instrumentation and experimental protocols as well as improved data handling. Yet, there is room for improvement and the subject addressed here is a major factor that influences the intensities of the spectra, namely x-ray attenuation factors. The attenuation of intensity emissions is significantly affected by finite sample size. It is fair to say that nearly all XAS (XANES and XAFS) measurements reported in the literature neglect this factor. Allowing for this, makes possible the extraction of more accurate multiplicities which because of correlation also influences the Debye-Waller-type factors.

In the aforementioned paper [1], in which we give the integral expressions for calculating absorption factors relating to fluorescence emissions for finite homogeneous samples in the shapes of a cylinder and a sphere (for instance represented by a pendant drop as in solution studies) have been derived using procedures originally developed for the x-ray diffraction case. The integrals are easily computed numerically and these procedures can be easily applied to correct the experimental EXAFS spectra for sample attenuation due to geometry.

We have been granted beamtime in May 2013 on the Swiss-Norwegian Beamlines for setting up and testing experimental protocols for reference compounds. The intention is to refine the procedure for the convenience of the general user and which will further improve the value of EXAFS as a structural method.

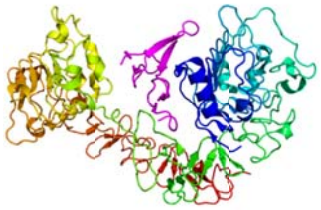
David G. Nicholson

[1]. H B Larsen, G Thorkildsen and D. G. Nicholson Phys. Scr. 86 (2012) 065601

The Fluoro-organic group: Cancer treatment by inhibition of epidermal growth factor tyrosine kinase

Introduction

Epidermal growth factor receptor tyrosine kinase (EGFR-TK) is one of the more important targets in small molecular cancer therapy.[1,2] These transmembrane enzyme-receptor complexes contain a binding site for external messenger molecules like epidermal growth factors (EGF), and an intracellular kinase domain.



Binding of EGF induces dimerization and thereby activation of the kinase domain.[2] Monoclonal antibodies such as Cetuximab and Panitumumab are efficient in blocking the entrance of EGF to EGFR,[3, 4] and some monoclonal antibodies might in addition trigger immune responses.[1, 5] Properly designed low molecular weight compounds are on the other hand attractive as inhibitors of the intracellular kinase domain due to their more moderate cost profile.

Organic chemistry

With the goal of discovering new active compounds for inhibition of EGFR, and to understand structure activity relationships we are building molecules based on three different scaffolds: pyrrolopyrimidines, thienopyrimidines and furopyrimidines. Although, not looking too different, both the bond length in the 5-membered ring and the hydrogen bonding ability of the pyrrol affects ligand binding to the biological target.

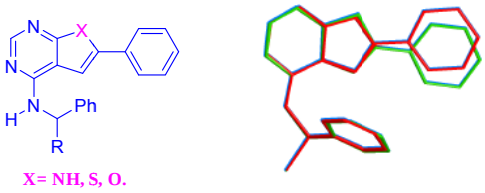
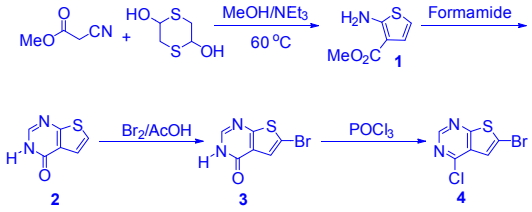


Figure 1. *Core structures investigated and effect of heteroatom on position of the 6-aryl ring.*

A key point in the optimisation phase is to have robust chemistry to late stage intermediates, so a high number of derivatives can be made with minimal effort. Thereby, we more efficiently can tune both drug-receptor interactions and improve the "drugability" of the molecules. For the thienopyrimidines efforts have been put into designing robust large scale processes towards the versatile building block **4** (Scheme 1). Now all steps can be performed on a 100 grams scale without chromatography.



Scheme 1. *Route to the basic core of thienopyrimidine **4** used for grafting suitable substituents.*

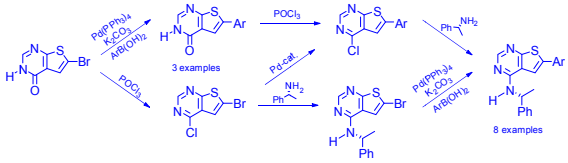
Scale up of synthesis

Purification by crystallisation

Scale-up Queen Ellen M. Skjønsfjell (Master student)

Figure 2. *Scale process to the thienopyrimidine core.*

Starting from compound **4**, we have further studied route selection strategies, and optimisation of Suzuki couplings with aryl boronic acids.[6]



Scheme 2. *Transformations on thienopyrimidines*

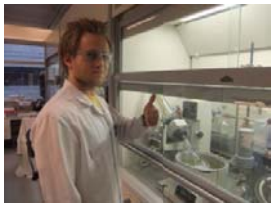
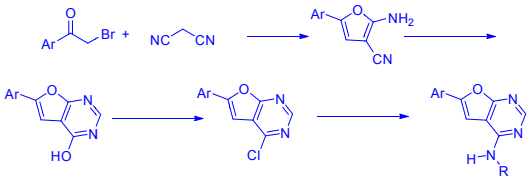


Figure 3. *PhD student Steffen Bugge after a successful Suzuki coupling.*

The chemical routes to the pyrrolopyrimidines,[7, 8] and furopyrimidines (Scheme 3) are suitable production processes. However, the methods are less attractive for creating an extended library of compounds. Therefore, the group is developing new strategies towards these scaffolds.



Scheme 3. *Route currently used for the furopyrimidines.*

Molecular docking

To create working hypothesis, and as an aid to explain structure activity relationships we use molecular modelling. Figure 4 shows one of the thienopyrimidine in the ATP binding site of EGFR.

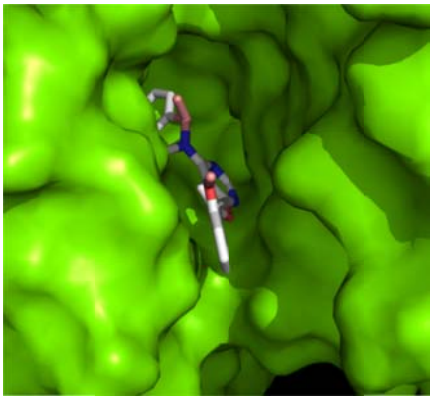


Figure 4. *A thienopyrimidine docked in the EGFR-TK ATP binding domain.*

In vitro testing towards kinases

All the prepared compounds are tested for their ability to inhibit EGFR (ErbB1) tyrosine kinase activity. This is done as 10 point titration in duplicates (purchased from Invitrogen) at various ATP concentrations.

Kaspersen *et al.*[8] reported our first study on EGFR inhibitors, where we identified eight new compounds having IC_{50} values in the range of 2.8-9.0 nM. The structure activity relationships identified are shown in Figure 5.

Five of these had a fluorine atom positioned at sites susceptible to oxidative metabolism. *In vitro* experiments with liver microsomes showed that fluoro insertion halts metabolism. Surprisingly, we later discovered that this compound class with a different substitution pattern had activity towards protozoas.

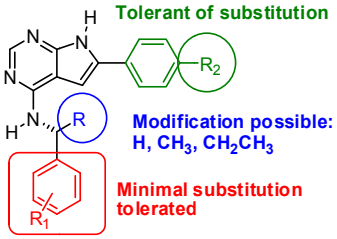


Figure 5. *Effect of structural variation on EGFR-TK activity.*

We have now profiled thienopyrimidines for the same application, and an invention is currently under evaluation for patenting.

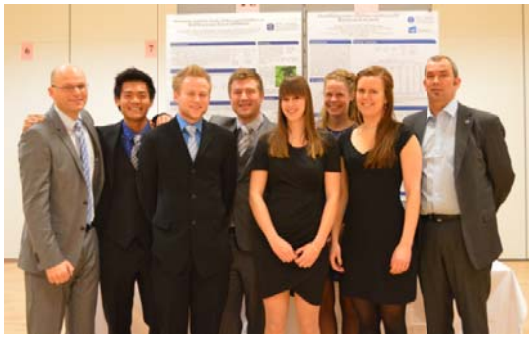


Figure 6. *Kinase team members at Organic Chemistry Meeting, Skeikampen 2013.*

Acknowledgement

Professor Geir Bjørkøy (St. Olavs/HIST) and co-workers is acknowledged for taking on the cell studies. Anders Jahres foundation is acknowledged for financial support.

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Bård Helge Hoff

Swiss-Norwegian Beamlines: Crystal and electronic structures of silver sulphate measured over an extended temperature range: a combined single crystal and EXAFS study

Despite the department and faculty entering an extended period of austerity until 2015 we are still able to make full use of the facilities of the Swiss-Norwegian Beamlines at the European Synchrotron Radiation Facility in Grenoble because this activity is pretty well ring-fenced by contract. So, no need for us at least to metaphorically re-use teabags.

The project described here is part of a wider research collaboration with the Department of Mathematics and Natural Science, University of Stavanger in connection with my role there as Visiting Professor. The project is an ongoing experimental study on the temperature-dependent properties silver sulphate.

Introduction

Silver sulphate, Ag2SO4, is a potential metal/metal sulphate reference electrode in solid state electrochemical SO2 gas sensors [1]. The material exhibits high cationic conductivity, which is interesting given the size of silver cations and the fact that the mechanism behind the process is not fully understood [1]. Any rationale of the mechanism must be based on the crystal structure. The literature shows that there is a general assumption that the structure of silver sulphate is known, and with good reason because the structure was reported as far back as 1931 [2]. Over the years, a number of studies have relied on this crystal structure. An example is the seminal spectroscopic study [4] on the colour of silver chromate incorporated into silver sulphate, the interpretation of which relies on the structure.

Unfortunately, these studies can be likened to castles built on sand because assumed structure from 1931 is simply wrong [3]. Current state of the art measurements using the facilities of the Swiss-Norwegian Beamlines (SNBL) will also parameters other than accurate atomic positions that are necessary in studies on the sensor properties of silver sulphate.

Preliminary results
Crystals of Ag2SO4 have been grown in an environment that nullifies the influence of gravity. By these means we have acquired well-formed crystals that range in size from the sub-millimeter to several millimeters.

We wished to exploit the combined power of synchrotron X-ray spectroscopy and diffraction on single crystals at low temperatures as well as around the phase transition temperature. The first sets of measurements at SNBL were carried out in 2012 and continuation experiments will be performed in May 2013.

The combination of techniques at SNBL also made it possible to measure the atomic displacement parameters as represented by MSRD (mean square relative displacement) which gives rise to the temperature-dependent damping factor in EXAFS) and MSD (mean square displacement which is represented by the Debye-Waller factors), respectively [4]. We have a choice of crystals with dimensions that are amenable to spectroscopy and to the various diffraction methods (allowing us to take into consideration the effects of absorption and extinction). At this stage, we have observed interesting temperature effects some of which are consistent with disproportionation.

Future work.—Next year´s (2013) powder diffraction measurements on will centre on the question of whether or not there is disproportionation because knowing this is critical for rationalising the temperature–dependent properties. Measurements on single crystals will enable us us to look at the directional dependence of the EXAFS. A full data set at a given temperature would yield the accurate crystal structure while diffraction data collected over a series of temperatures would give uncorrelated MSDs.

In addition, EXAFS will be measured on crystals that have been damaged by deliberate overexposure to radiation (at the Ag-K-edge, 25.5 keV) in order to study Ag/AgO-clustering. Progressive reduction can be followed by edge shifts. The cluster size can be estimated by the correlation between the averaged nearest metal neighbours in the first metal-metal shell.

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David G. Nicholson

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A copper bar from Røros copper works. © K.Glavatskiy

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Model of an old copper mine. © K.Glavatskiy

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Zeeshan, Muhammad; Sliwka, Hans-Richard; Partali, Vassilia; Martinez, Ana.
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Honours, Extracurricular activities, Participation in Courses, Conferences, Lectures, and Study Visits

B. Alsberg

Section Leader, Applied Theoretical Chemistry Group, Department of Chemistry, NTNU.

''95th Canadian Chemistry Conference and Exhibition'', Calgary, AB Canada, 2012-05-26 - 2012-05-30
Co-Author of Lecture on: ''Theory-assisted design of homogeneous catalysts: New strategies''.

Conference ''The 11th Annual Meeting on High Performance Computing and Infrastructure for computational science in Norway'', Tromsø, Norway, 2012-06-14 - 2012-06-15
Co-Author of Poster on: ''DENOPTIM: De novo OPTimization of Inorganic Molecules''.

''The XXV International Conference on Organometallic Chemistry'', Lisbon, Portugal, 2012-09-02 - 2012-09-07
Co-Author of Poster on: ''DENOPTIM: De novo OPTimization of Inorganic Molecules''.

Pedestrian shopping street in Røros. © K.Glavatskiy

D. Bedeaux

''CECAM Wokshop on Structure, functionalization and dynamics of fluid interfaces'', Zaragosa, Spain, 2012-10-14 - 2012-10-17
Co-Author of Lecture on: ''Non-Equilibrium Thermodynamics for surfaces; Local Equilibrium; The Square Gradient Theory''.

Conference ''High Power Computing'', Trondheim, Norway, 2012-05-10
Co-Author of Lecture on: ''Large and small system thermodynamic properties from molecular dynamics simulations''.

''XXIII Sitges Conference: Understanding and Managing Randomness in Physics, Chemistry and Biology'', Barcelona, Spain, 2012-06-03 - 2012-06-08
Co-Author of Lectures on: ''Time correlation functions for fluids in mesoscopic systems'' and ''Connections between small and large systems' thermodynamics''.

''18th Symposium on Thermophysical properties'', Boulder, CO USA, 2012-06-24 - 2012-06-29
Co-Author of Lectures on: ''Non-Equilibrium Thermodynamics'' and ''Assessing the Coupled Heat and Mass Transport of Hydrogen through a Palladium Membrane''.

''IWNET 2012 6th International Workshop on Nonequilibrium Thermodynamics and 3rd Onsager Symposium'', Røros, Norway, 2012-08-19 - 2012-08-24
Co-Author of Lectures on: ''Active transport of the calcium pump: Introduction of the temperature difference as a driving force'' and ''Predicting Fick and Maxwell-Stefan Diffusivities in Liquids''.

T. Berg

Sabbatical, autumn 2012.

Conference ''25th Task force meeting of the ICP vegetation'' Brescia, Italy, 2012-01-31 - 2012-02-02
Co-Author of Lecture on: ''Three decades of atmospheric metal deposition in Norway as evident from analysis of moss samples: Temporal trends and progress in 2010''.

P. Brandvik

Conference ''INTERSPILL 2012'', London, UK, 2012-03-12 - 2012-03-15
Co-Author of Lectures on: ''SINTEFs Oil Weathering Model Combined laboratory characterisation and field verification'' and ''Oil spills in ice Main operational differences compared to "ordinary" open water oil spills''.

Seminar ''Beredskapsforum 2012 (KLIF, OLF og KyV)'', Oslo, Norway, 2012-02-02
Co-Author of Lecture on: ''Undervannsdispergering - Erfaringer fra Mexicogulfen, behov for endringer i norsk beredskap?''.

''Oil In Ice - Fram Center Workshop'', Tromsø, Norway, 2012-01-23 - 2012-01-24
Co-Author of Lecture on: ''Fate processes important for oil-in-ice modeling Status and future R&D needs''.

Seminar ''Industry Technical Advisory Committee for oil spill response (ITAC)'', Southampton, UK, 2012-11-29 - 2012-11-30

Co-Author of Lecture on: ''Oil Spill R&D at SINTEF: Focusing on subsea releases and Arctic conditions''.

''EMSA Workshop addressing the Use of Oil Spill Dispersants'', Lisbon, Portugal, 2012-11-26 - 2012-11-27
Co-Author of Lecture on: ''Subsurface releases of oil: Oil droplet distributions and dispersant injection techniques''.

Seminar ''API Subsurface modelling work shop'', Houston, TX USA, 2012-10-24 - 2012-10-25
Co-Author of Lecture on: ''Evaluation of subsea dispersant injection methods, equipment and effectiveness''.

Seminar ''Dypvannsdispergeringsseminar (OLF)'', Oslo, Norway, 2012-02-03
Co-Author of Lecture on: ''Studies of oil droplet formation from subsea releases, with and without use of dispersants''.
Seminar ''Når ulykker truer miljøet 2012 - Klif/Petil'', Oslo, Norway, 2012-02-01
Co-Author of Lectureon: ''Undervannsdispergering, nye muligheter og utfordringer!''.

Conference ''GOMRI Kick-off seminar'', Port Aransas, TX USA, 2012-03-08 - 2013-03-09
Co-Author of Lecture on: ''SINTEF Scientific Participation in DROPPS: Experimental simulations and modelling of subsurface blowouts''.

Conference ''CRRC Dispersant Research Forum 2012'', Baton Rouge, LA USA, 2012-01-10 - 2012-01-11
Co-Author of Lecture on: ''SINTEF – R&D within: Oil weathering, Dispersant and Deep water blow-outs''.

Seminar ''Energieffektiv og miljøvennlig bærekraftig teknologi - OG21'', Tromsø, Norway, 2012-04-18
Co-Author of Lecture on: ''Oljevernberedskap i Barentshavet Status og utfordringer''.

S. Bugge

Conference ''Organisk kjemisk vintermøte 2012'', Skeikampen, Norway, 2012-01-12 - 2012-01-15
Co-Author of Lecture on: ''Route selection in synthesis of thienopyrimidines''.
Co-Author of Poster on: ''Building blocks for thienopyrimidines synthezised using microwave heating''.

O. Burheim

Conference ''Technoport RERC 2012'', Trondheim, Norway, 2012-04-15 - 2012-04-17
Co-Author of Lectures on: ''CAPMIX - Deploying capacitors for salinity difference power extraction'', ''New operation mode for Capacitive energy extraction based on Donnan Potential'', ''Fluid Mechanics of Salinity Difference Power Systems'', and ''A Method for determination of Ion Transference Numbers in Ion-Exchange Membranes for RED Applications''.

''International Work Shop on Salinity Gradient Energy'', Milan, Italy, 2012-09-04 - 2012-09-06
Author of Lecture on: ''Measuring Membrane Parameters for RED and CAPMIX Performance Analysis''.
Co-Author of Lectures on: ''Transport Phenomena in Auto Generative Capacitive Blue Energy Systems'', ''Effect of additional charging on the performance of Capacitiv energy extraction based on Donnan Potential'', ''Cylindrical Design for Blue Energy'', and ''Modelling direct electricity production by capacitive energy extraction from salinity gradients''.

Conference ''The Norwegian Chemical Society'', Trondheim, Norway, 2012-09-25 - 2012-09-25
Author of Lecture on: ''Salinity Gradient Energy – Renewable Chemical Energy''.

Conference ''World Hydrogen Fuel Cells'', 2012-06-03 - 2012-06-07
Co-Author of Lectures on: ''Thermal Conductivity in aged Porous Transport Layers (PTL/GDL) for PEMFC'' and ''Measured Temperature Profiles in a Hydrogen Hydrogen PEM Cell''.

''18th Symposium on Thermophysical properties'', Boulder, CO USA, 2012-06-24 - 2012-06-29
Co-Author of Lecture on: ''Non-Equilibrium Thermodynamics - a Tool for Fuel Cell Design''.

Conference: ''TMS 2012 Annual Meeting & Exhibition'', Orlando, FL USA, 2012-03-11 - 2012-03-15
Co-Author of Lecture on: ''A Solid State Thermoelectric Power Generator Prototype Designed to Recover Radiant Waste Heat''.

K.L. Bøyesen

''The 15th International Conference on X-ray Absorption Fine Structure'', Beijing, China, 2012-07-22 - 2012-07-28
Co-Author of Lecture on: ''Determination of the Synergistic Effect of Copper and Vanadium Deposited on AlPO-5 for the Formation of Acrolein''.

Conference ''Norwegian Synchrotron and Neutron User Meeting'', Stavanger, Norway, 2012-01-30 - 2012-01-31
Co-Author of Poster on: ''Study of the Synergistic Effect of Copper and Vanadium Deposited on Microporous Systems for the Selective Oxidation of Propene. -A combined in situ XAS/XRD study''.

N. Davari

''Annual meeting in computational chemistry'', Hamn i Senja, Norway, 2012-06-12 - 2013-06-13
Co-Author of Lecture on: ''Ionization potential and excitation energy of molecules in high electric fields''.

A. Fiksdahl

Conference ''Organisk Kjemisk Vintermøte'', Skeikampen, Norway, 2012-01-12 - 2012-01-15
Co-Author of Posters on: ''Gold(I)Catalyzed Dimerization of vinyl amides'' and ''Gold(I)-Catalyzed Dimerization of vinyl compounds''.
Co-Author of Lecture on: ''Gold(I)-Catalyzed Cyclization of Propargyl Substrates''.

Conference ''Organikardagarna XXIII'', Gothenburg, Sweden, 2012-06-12 - 2012-06-15
Author of Lecture on: ''Golden triple bonds''.

Det Kongelige Norske Vitenskabers Selskab, DKNVS, Meeting, Trondheim, Norway, 2012-02-20
InvitedLecture on: ''Gullkatalyse i organisk syntese''.

''Ny gullalder i kjemien''. Interview on Internet, forskning.no, 2012-10-30

''Int. Symposia on Advancing the Chemical Sciences'', Edinburg, Germany, 2012-06-12 - 2012-06-15
Co-Author of Poster on: ''Gold(I) Catalyzed Cycloaddition Reactions of Propargyl Substrates''.

T. P. Flaten

Editor, Norsk Epidemiologi ((Norwegian Journal of Epidemiology)

Board member, The Committee for Geomedicine of the Norwegian Academy of Science and Letters
Board member, Norwegian Chemical Society, Trondheim Branch

Board member, Programme board for Environmental Exposures and Health Outcomes, The Norwegian Research Council.

Councilor, International Society for Trace Element Research in Humans (ISTERH)

S. Forselv

Conference ''15th Nordic Symposium on Catalysis'', Norway, 2012-06-10 - 2012-06-12
Co-Author of Poster on: ''New Insights on UiO MOFs by Variable Temperature DR-FTIR''.

Conference ''MOF 2012'', Edinburgh, UK, 2012-09-16 - 2012-09-19
Co-Author of Poster on: ''New Insights on Zr-UiO-MOFs by Variable Temperature DRIFTS''.

O.R. Gautun

Meeting ''Motivasjonsforedrag for Høiskolens Chemikerforening ved NTNU'', Trondheim, Norway, 2012-11-09
Author of Lecture on: ''Molekyler som endret verden''.

Conference: ''Organisk Kjemisk Vintermøte'', Skeikampen, Norway, 2012-01-12 - 2012-01-15
Organizer of ''Organisk Kjemisk Vintermøte'', Skeikampen, Norway 2012-01-12 – 2012-01-15.

Member of NFRs Committee for Marine Bioprospecting and Organic Synthesis.

Co-Author of Poster on: ''Studies Towards the Synthesis of Potential Selective Inhibitors of Tyrosine Kinase 2''.

K.F. Gebremariam

Conference ''ICCE22 ERICE11'', Roma, Italy, 2012-07-15 - 2012-07-20
Co-Author of Lecture on: ''Revisiting the Daniell Cell''.

A. Gerontas

Conference: ''8th meeting of STEP'', Corfu, Greece, 2012-06-21 - 2012-06-24
Co-Author of Lecture on: ''The first steps of the High Performance Liquid Chromatography (HPLC) instrumentation: Discussing the Role of the Press in the dissemination of analytical technology at the end of the 1960s and early 1970s''.

Research stay; Doan Fellow 2012 in the Chemical Heritage Foundation, Philadelphia, PA, USA; February-June 2012.

Conference ''4th EUCheMS Congress'', Praha, Czech Republic, 2012-08-26 - 2012-12-30

K. Glavatskyy

''CECAM Wokshop on Structure, functionalization and dynamics of fluid interfaces'', Zaragosa, Spain, 2012-10-14 - 2012-10-17
Co-Author of Lecture on: ''Non-Equilibrium Thermodynamics for surfaces; Local Equilibrium; The Square Gradient Theory''.

''18th Symposium on Thermophysical properties'', Boulder, CO USA, 2012-06-24 - 2012-06-29
Co-Author of Lecture on: ''Non-Equilibrium Thermodynamics - a Tool for Fuel Cell Design''.

''IWNET 2012 6th International Workshop on Nonequilibrium Thermodynamics and 3rd Onsager Symposium'', Røros, Norway, 2012-08-19 - 2012-08-24

J. Han

Conference ‘’Organisk kjemisk vintermøte 2012’’, Skeikampen, Norway, 2012-01-12 - 2012-01-15
Co-Author of Poster on: ‘’Investigation into the synthesis of 2-aminopyrroles’’

E. Hjertenes

Norweigan Chemical Society - Annual meeting in the computational chemistry; 2012-06-12 - 2012-06-13
Author of lecture on: "Benchmark data and DFT evaluation for sodium-graphite interactions: DFT in DuraMat".

Sostrup Summer School in Quantum Chemistry and Molecular Properties; 2012-07-01 - 2012-07-13
Author of Poster on: "Non-orthogonal Slater Determinants - NOSD".

B.H. Hoff

Section Leader, Organic Chemistry Group, Department of Chemistry, NTNU.

Conference ‘’Organisk kjemisk vintermøte 2012’’, Skeikampen, Norway, 2012-01-12 - 2012-01-15

Co-Author of Lecture on: ‘’Route selection in synthesis of thienopyrimidines’’ and ‘’In vitro testing of pyrrolopyrimidines as kinase inhibitors’’.
Co-Author of Posters on: ‘’Investigation into the synthesis of 2-aminopyrroles’’ and ‘’Building blocks for thienopyrimidines synthezised using microwave heating’’.

Conference ‘’Technoport 2012’’, Trondheim, Norway, 2012-04-16 - 2012-04-18
Co-Author of Poster on: ‘’Organosolv pretreatment of biomass for biofuel and biorefinery applications’’

Co-Author of Lecture on: ‘’Hot water extraction of hemicellulose from spruce and bagasse by use of microwave heating’’.
Co-Author of Poster on: ‘’Hot water extraction of hemicellulose from softwood and sugarcane bagasse using microwave heating technology’’.

‘’4th Nordic Wood Biorefinery Conference in Helsinki’’, Helsinki, Finland, 2012-10-23 - 2012-10-25

N. Iqbal

Conference ‘’Organisk Kjemisk Vintermøte’’, Skeikampen, Norway, 2012-01-12 - 2012-01-15
Co-Author of Posters on: ‘’Gold(I)Catalyzed Dimerization of vinyl amides’’ and ‘’Gold(I)-Catalyzed Dimerization of vinyl compounds’’.
Co-Author of Lecture on: ’’Gold(I)-Catalyzed Cyclization of Propargyl Substrates’’.

‘’Int. Symposia on Advancing the Chemical Sciences’’, Edinburg, Germany, 2012-06-12 - 2012-06-15
Co-Author of Poster on: ‘’Gold(I) Catalyzed Cycloaddition Reactions of Propargyl Substrates’’.

Souvenirs from Røros. . © K.Glavatskiy

E. Jacobsen

Conference: ‘’7th CeBiTec Symposium: Bio-integrated Organic Synthesis in Industry’’, Bielefeld, Germany, 2012-12-16 - 2012-12-19
Author of Lecture on: ‘’Antiepileptic drug (R)-Stiripentol’’.
Co-Author of Poster on: ‘’Synthesis of chiral drugs by Candida antarctica lipase A catalysis’’.

S.J. Kaspersen

Conference ‘’Organisk kjemisk vintermøte 2012’’, Skeikampen, Norway, 2012-01-12 - 2012-01-15
Co-Author of Lectures on: ‘’Route selection in synthesis of thienopyrimidines’’ and ‘’In vitro testing of pyrrolopyrimidines as kinase inhibitors’’.
Co-Author of Poster on: ‘’Investigation into the synthesis of 2-aminopyrroles’’.

S. Kjelstrup

Sabbatical, autumn 2012.

‘’CECAM Wokshop on Structure, functionalization and dynamics of fluid interfaces’’, Zaragosa, Spain, 2012-10-14 - 2012-10-17
Co-Author of Lecture on: ‘’Non-Equilibrium Thermodynamics for surfaces; Local Equilibrium; The Square Gradient Theory’’.

Conference ‘’High Power Computing’’, Trondheim, Norway, 2012-05-10
Co-Author of Lecture on: ‘’Large and small system thermodynamic properties from molecular dynamics simulations’’.

''XXIII Sitges Conference: Understanding and Managing Randomness in Physics, Chemistry and Biology'', Barcelona, Spain, 2012-06-03 - 2012-06-08
Co-Author of Lectures on: ''Time correlation functions for fluids in mesoscopic systems'' and ''Connections between small and large systems' thermodynamics'' and ''Connections between small and large systems' thermodynamics''.

Conference ''World Hydrogen Fuel Cells'', 2012-06-03 - 2012-06-07
Co-Author of Lectures on: ''Thermal Conductivity in aged Porous Transport Layers (PTL/GDL) for PEMFC'' and ''Measured Temperature Profiles in a Hydrogen Hydrogen PEM Cell''.

''Symposium on thermodynamics and transport processes'', Sevilla, Spain, 2012-02-12 - 2012-02-13
Author of Lecture on: ''Coupled transport of heat and mass at surfaces''.

Debate ''Åpent debattmøte om fremtidens FRIPRO'', Bergen, Norway, 2012-05-10
Debate on ''De leveringsdyktige eller de dristige prosjektene?''.

''Fuel Cell System Group Meeting TU Delft'', Delft, Netherlands, 2012-01-17
Author of Lecture on: ''Energy efficient design targeting the polymer electrolyte fuel cell''.

Meeting '' Høytidsmøtet DKNVS'', trondheim, Norway, 2012-03-09
Author of Lecture on: ''John Ugelstad (1921-1997) til minne''.

Meeting ''Fredagskollokvium'', Trondheim, Norway, 2012-08-31
Author of Lecture on: ''Thermodynamics for the nanoscale''.

Conference ''Mexican XXVII Congress of Thermodynamics, Toluca, Mexico, 2012-09-10 - 2012-09-14
Author of Lecture on: ''Thermodynamics of small systems''.

''IWNET 2012 6th International Workshop on Nonequilibrium Thermodynamics and 3rd Onsager Symposium'', Røros, Norway, 2012-08-19 - 2012-08-24
Co-Author of Lecture on: ''Active transport of the calcium pump: Introduction of the temperature difference as a driving force''.

Conference ''Technoport RERC 2012'', Trondheim, Norway, 2012-04-15 - 2012-04-18
Co-Author of Lecture on: ''A Method for determination of Ion Transference Numbers in Ion-Exchange Membranes for RED Applications''.

Conference: ''TMS 2012 Annual Meeting & Exhibition'', Orlando, FL USA, 2012-03-11 - 2012-03-15
Co-Author of Lecture on: ''A Solid State Thermoelectric Power Generator Prototype Designed to Recover Radiant Waste Heat''.

Conference ''Nasjonal Konferanse for Materialteknologi'', Trondheim, Norway, 2012-05-09 - 2012-05-10
Co-Author of Lecture on: ''Eksergianalyse av silisiumproduksjonsprosessen''.

''The 25th International Conference on Efficiency, Cost, Optimization Simulation and Environmental Impact of Energy Systems, ECOS 2012'', Perugia, Italy, 2012-06-26 - 2012-06-29
Co-Author of Lectures on: ''Exergy Analysis of the Silicon Production Process'' and ''Evaluation of the Oil and Gas Processing at a Real Production Day on a North Sea Oil Platform Using Exergy Analysis''.

N. Klausen

''Researchers night, 2012'', Trondheim, Norway, 2012-09-27
Co-Author of Lecture on: ''Knallforelesning i kjemi''.

H. Koch

Sabbatical, autumn 2012.

Norweigan Chemical Society - Annual meeting in the computational chemistry; 2012-06-12 - 2012-06-13
Co-author of lecture on: "Benchmark data and DFT evaluation for sodium-graphite interactions: DFT in DuraMat".

Sostrup Summer School in Quantum Chemistry and Molecular Properties; 2012-07-01 - 2012-07-13
Co-author of poster on: "Non-orthogonal Slater Determinants - NOSD".

T. Kristiansen

''XAFS15: The 15th International Conference on X-ray Absorption Spectroscopy'', Beijing, China, 2012-08-22 - 2012-08-30
Co-Author of Lecture on: ''There and back again: The unique nature of copper in APD-silica aerogels''.

Conference ''Norwegian Synchrotron and Neutron User Meeting'', Stavanger, Norway, 2012-01-30
Co-Author of Lecture on: ''XAS In Situ studies on Size and Shape Selectivity of Copper Nanoparticles in Silica Gels: Aerogels Vs. Xerogels''.

L. Kvittingen

Conference ''ICCE22 ERICE11'' Roma, Italy, 2012-07-15 - 2012-07-20
Co-Author of Lecture on: ''Revisiting the Daniell Cell''.

''Reseachers Night'', Trondheim, Norway, 2012-10-19
Co-Author of Poster on: ''Nytt gammelt glass. Laboratorieutstyr anno 1550''.

Meeting ''MUBIL - prosjekt ved Gunnerus'' 2012-11-12
Co-Author of Lecture on: ''Rekonstruksjon av destillasjon fra Adam Lonicers Kreuterbuch 1557''.

Meeting '' Kjemien Stemmer '', Oslo, Norway, 2012-05-10
Co-Author of Lecture on: ''Fortidens samlinger i dagens kurs''.

A. Lervik

''IWNET 2012 6th International Workshop on Nonequilibrium Thermodynamics and 3rd Onsager Symposium'', Røros, Norway, 2012-08-19 - 2012-08-24
Co-Author of Lecture on: ''Active transport of the calcium pump: Introduction of the temperature difference as a driving force''.

S. Lierhagen

''4th Norwegian Environmental Toxicology Symposium'', Tromsø, Norway, 2012-10-16 - 2012-10-18
Co-Author of Poster on: ''Differences in concentrations of pollutants in common eiders from the Baltic Sea and Svalbard''.

A. Lykknes

Conference ''8th meeting of STEP'', Corfu, Greece, 2012-06-21 - 2012-06-24
Co-Author of Lecture on: ''The first steps of the High Performance Liquid Chromatography (HPLC) instrumentation: Discussing the Role of the Press in the dissemination of analytical technology at the end of the 1960s and early 1970s''.

''Skandale om kjemisamlingen forsvinner''. Interview for Newspaper Universitetsavisa, Trondheim, Norway, 2012-03-20

''5th International Conference of the ESHS'', Athen, Greece, 2012-11-01 - 2012-11-03
Co-Author of Lectures on: ''Symposium: Women in the Laboratory from Early Modern Times to the 20th Century'' and ''The Wife as Risk-Taker and Conceptual Thinker: Ida Noddack-Tacke and Nuclear Fission''

Conference ''Seventh British-North American joint meeting of the BSHS, CSHPS, and HSS''. Philadelphia, PA USA, 2012-07-11 - 2012-07-14
Co-Author of Lecture on: ''Ida Noddack and the Fission Proposal: The Actor's Perspective''.

Research stay at the European Synchrotron Radiation Factility (ESRF), Swiss-Norwegian Beam Line, Grenoble, France, 22-25 May, 2012

Member of the Sientific Committee of the 8th Meeting of STEP (Science and Technology in the European Periphery), Corfu, Greece, 21-24 June, 2012.

Member of the Scientific Committee of the 9th International Conference on the History of Chemistry, to be held in Uppsala, Sweden, 21-23 August, 2013

Conference 4th EuCheMS Congress, Prague, Czech Republic, 26-30 August, 2012

Vice chair and web editor of the Working Party on the History of Chemistry, EuCheMS

Board member of the Commission on the History of Women in Science, Technology and Medicine, of the International Union for the History of Science, Technology and Medicine, Division of History of Science and Technology

Board member and secretary of the History of Chemistry Group of the Norwegian Chemical Society

M. Martinsen

''60th ASMS Conference on Mass Spectrometry and Allied Topics'', Vancouver, BC Canada 2012-05-20 - 2012-05-24
Co-Author of Lecture on: ''Real time visualization of spatially and temporally resolved data from an in-field, mobile membrane introduction mass spectrometer''.

Co-Author of Poster on: ''The Use of Multivariate Analysis as a Fingerprinting Tool for Membrane Introduction Mass Spectrometry (MIMS) Data from Crude Hydrocarbon Samples''.

K. Mathisen

''The 15th International Conference on X-ray Absorption Fine Structure'', Beijing, China, 2012-07-22 - 2012-07-28
Co-Author of Lecture on: ''Determination of the Synergistic Effect of Copper and Vanadium Deposited on AlPO-5 for the Formation of Acrolein''.

Conference ‘’Norwegian Synchrotron and Neutron User Meeting’’, Stavanger, Norway, 2012-01-30 - 2012-01-31
Co-Author of Posters on: ‘’Study of the Synergistic Effect of Copper and Vanadium Deposited on Microporous Systems for the Selective Oxidation of Propene. -A combined in situ XAS/XRD study’’, ‘’Characterization of gold and copper nanoparticles in mesoporous frameworks using of X-ray absorption spectroscopy’’, ‘’Stabilisation of trivalent vanadium in zeotypic systems’’ and ‘’Characterization of hierarchical SAPO-34 from one pot synthesis; bimodal pore distribution affects sintering process of metallic nanoclusters’’.

‘’XAFS15: The 15th International Conference on X-ray Absorption Spectroscopy’’, Beijing, China, 2012-08-22 - 2012-08-30

Co-Author of Lecture on: ‘’There and back again: The unique nature of copper in APD-silica aerogels’’.
Author of Lecture on: ‘’Utilisation of XAS in mixed chemical environments for catalytic red-ox applications’’.

Conference ‘’Norwegian Synchrotron and Neutron User Meeting’’, Stavanger, Norway, 2012-01-30
Co-Author of Lecture on: ‘’XAS In Situ studies on Size and Shape Selectivity of Copper Nanoparticles in Silica Gels: Aerogels Vs. Xerogels’’.

Conference ‘’2nd National Meeting on Inorganic and Materials Chemistry’’, Norway, 2012-10-12 - 2012-10-13
Author of Lecture on: ‘’Nanoparticles in porous materials; preparation and applications’’.

S. Melnes

Conference: ‘’Det 27. Organisk Kjemiske Vintermøte’’, skeikampen, Norway, 2012-01-12 - 2012-01-15
Co-Author of Poster on: ‘’Studies Towards the Synthesis of Potential Selective Inhibitors of Tyrosine Kinase 2’’.

Ø. Mikkelsen

Deputy Head of the Department of Chemistry.

Section Leader, Analytical and Environmental Chemistry Group, Department of Chemistry, NTNU.

‘’60th ASMS Conference on Mass Spectrometry and Allied Topics’’, Vancouver, BC Canada, 2012-05-20 - 2012-05-24
Co-Author of Lecture on: ‘’Real time visualization of spatially and temporally resolved data from an in-field, mobile membrane introduction mass spectrometer’’.
Co-Author of Poster on: ‘’The Use of Multivariate Analysis as a Fingerprinting Tool for Membrane Introduction Mass Spectrometry (MIMS) Data from Crude Hydrocarbon Samples’’.

D.G. Nicholson

Sabbatical, spring and autumn 2012.

Conference ‘’Norwegian Synchrotron and Neutron User Meeting’’, Stavanger, Norway, 2012-01-30
Co-Author of Lecture on: ‘’XAS In Situ studies on Size and Shape Selectivity of Copper Nanoparticles in Silica Gels: Aerogels Vs. Xerogels’’.

‘’PSI seminar’’, Villigen, Switzerland, 2012-06-06
Co-Author of Lecture on: ‘’Single crystal diffraction and FLEXAFS -- complementary opprotunities’’.

M.- L. Olivier

Head of the Department of Chemistry.

V. Partali

‘’International conference’’, Versailles, France, 2012-10-24 - 2012-10-28
Co-Author of Poster on: ‘’Novel carotenoi lipid vectors for ocular gene therapy’’.

Patent no.: US Appl. 61.721.975 Registered 2012-11-02
Co-Author on ‘’Novel cationic carotenoid-based lipids as tracking agents for cellular nucleic acid uptake’’.

Annual meeting, "Cationic lipids as gene carriers", Doha, Qatar, 2012-11-08 - 2012-11-17
Presentation,"Cationic lipids based on highly unsaturated conjugated fatty acids", Doha, Qatar 2012-11-15

K. Sandbakk

Conference ‘’Technoport RERC 2012’’, Trondheim, Norway, 2012-04-15 - 2012-04-17
Co-Author of Lecture on: ‘’A Method for determination of Ion Transference Numbers in Ion-Exchange Membranes for RED Applications’’.

R. Schmid

‘’60th ASMS Conference on Mass Spectrometry and Allied Topics’’, Vancouver, BC Canada 2012-05-20 - 2012-05-24
Co-Author of Lecture on: ‘’Real time visualization of spatially and temporally resolved data from an in-field, mobile membrane introduction mass spectrometer’’.
Co-Author of Poster on: ‘’The Use of Multivariate Analysis as a Fingerprinting Tool for Membrane Introduction Mass Spectrometry (MIMS) Data from Crude Hydrocarbon Samples’’.

Conference ‘’20. Norske symposium i kromatografi’’, Sandefjord, Norway, 2012-01-08 - 2012-01-10
Co-Author of Poster on: ‘’Comprehensive Two-Dimensional Gas Chromatography’’.

R. Skorpa

‘’18th Symposium on Thermophysical properties’’, Boulder, CO USA, 2012-06-24 - 2012-06-29
Co-Author of Lecture on: ‘’Assessing the Coupled Heat and Mass Transport of Hydrogen through a Palladium Membrane’’.

E. Steinnes

‘’6th International Workshop on Biomonitoring of Atmospheric Pollution’’, Cesme, Turkey, 2012-10-15 - 2012-10-19
Author of Lecture on: ‘’Atmospheric deposition of pollutants studied by moss sampling: Experience from 35 years of monitoring in Norway (keynote lecture)’’.

‘’16. International Conference on Heavy Metals in the Environment’’, Roma, Italy, 2012-09-23 - 2012-09-27
Author of Lecture on: ‘’Heavy metal contamination of the terrestrial environment from long-range atmospheric transport: Evidence from 35 years of research in Norway’’.

View from Røros copperworks. © K.Glavatskiy

‘’6th International Symposium on In Situ Nuclear Metrology as a Tool for Radioecology’’, Brussels, Belgium, 2012-06-11 - 2012-06-15
Author of Lecture on: ‘’Importance of chemical speciation in assessing transfer of radionuclides in the environment’’.

‘’The 5th International Conference on Ecological Chemistry’’, Chisinau, Moldova, 2012-03-02 - 2012-03-04
Author of Lecture on: ‘’Three decades of atmospheric metal deposition in Norway as evident from analysis of moss samples’’.

Seminar ‘’25th Task force meeting of the ICP vegetation’’, Brescia, Italy, 2012-01-31 - 2012-02-02
Co-Author of Lecture on: ‘’Three decades of atmospheric metal deposition in Norway as evident from analysis of moss samples: Temporal trends and progress in 2010’’.

‘’International Seminar on Interactions of Neutrons with Nuclei’’, Alushta, Ukraine, 2012-05-21 - 2012-05-26
Co-Author of Lecture on: ‘’Mixed metal pollution from smelter industries studied by moss biomonitoring, INAA and ICPMS: Mo i Rana (Norway) case study’’.

Conference ‘’4th EUCheMS Congress’’, Praha, Czech Republic, 2012-08-26 - 2012-12-30

M. Takla

‘’18th Symposium on Thermophysical properties’’, Boulder, CO USA, 2012-06-24 - 2012-06-29
Co-Author of Lectures on: ‘’Assessing the Coupled Heat and Mass Transport of Hydrogen through a Palladium Membrane’’.

Conference: ‘’TMS 2012 Annual Meeting & Exhibition’’, Orlando, FL USA, 2012-03-11 - 2012-03-15
Co-Author of Lecture on: ‘’A Solid State Thermoelectric Power Generator Prototype Designed to Recover Radiant Waste Heat’’.

Conference ’’Nasjonal Konferanse for Materialteknologi’’, Trondheim, Norway, 2012-05-09 - 2012-05-10
Co-Author of Lecture on: ’’Eksergianalyse av silisiumproduksjonsprosessen’’.

‘’The 25th International Conference on Efficiency, Cost, Optimization Simulation and Environmental Impact of Energy Systems, ECOS 2012’’, Perugia, Italy, 2012-06-26 - 2012-06-29
Co-Author of Lectures on: ‘’Exergy Analysis of the Silicon Production Process’’.

T. K. Thvedt

Conference ‘’Organisk kjemisk vintermøte 2012’’, Skeikampen, Norway, 2012-01-12 - 2012-01-15
Co-Author of Poster on: ‘’Building blocks for thienopyrimidines synthezised using microwave heating’’.

T. Trinh

‘’XXIII Sitges Conference: Understanding and Managing Randomness in Physics, Chemistry and Biology’’, Barcelona, Spain, 2012-06-03 - 2012-06-08
Co-Author of Lecture on: ‘’Time correlation functions for fluids in mesoscopic systems’’.

T. Van Erp

Conference ''IWNET 2012: 6th International Workshop on Nonequilibrium Thermodynamics and 3rd Lars Onsager Symposium'' Røros, Norway, 2012-08-19 - 2012-08-24
Author of Lecture on: ''Dynamical Rare event simulation techniques for equilibrium and non-equilibrium systems''.

Workshop ''Modelling the Dynamics of Complex Molecular Systems'', Leiden, Netherlands, 2012-08-13 - 2012-08-17
Author of Lecture on: ''Dynamical rare event simulation techniques for equilibrium and non-equilibrium systems''.

V. Venkatraman

''The 11th Annual Meeting on High Performance Computing and Infrastructure for computational science in Norway'', Tromsø, Norway, 2012-06-14 - 2012-06-15
Co-Author of Poster on: ''DENOPTIM: De novo OPTimization of Inorganic Molecules''.

''The XXV International Conference on Organometallic Chemistry'', Lisbon, Portugal, 2012-09-02 - 2012-09-07
Co-Author of Poster on: ''DENOPTIM: De novo OPTimization of Inorganic Molecules''.

M. Voldsund

''18th Symposium on Thermophysical properties'', Boulder, CO USA, 2012-06-24 - 2012-06-29
Co-Author of Lectures on: ''Non-Equilibrium Thermodynamics'' and ''Assessing the Coupled Heat and Mass Transport of Hydrogen through a Palladium Membrane''.

''The 25th International Conference on Efficiency, Cost, Optimization Simulation and Environmental Impact of Energy Systems, ECOS 2012'', Perugia, Italy, 2012-06-26 - 2012-06-29

Co-Author of Lecture on: ''Evaluation of the Oil and Gas Processing at a Real Production Day on a North Sea Oil Platform Using Exergy Analysis''.

P. – O. Åstrand

''Annual meeting in computational chemistry'', Hamn i Senja, Norway, 2012-06-12 - 2013-06-13
Co-Author of Lecture on: ''Ionization potential and excitation energy of molecules in high electric fields''.

Leader of the Division of Computational Chemistry, Norwegian Chemical Society

Patent application no WO/2012/16403. Published 06.12.2012.
Coauthor on "Dielectric fluids having reduced streamer speed"

Leader of NTNU advisory committee on Computational Science and Visualization

Member of NTNU/SINTEF work group on Computational Science and Engineering

Member of Faculty Research Committee, Faculty of Natural Sciences and Technology, NTNU

Small waterfall in Hyttelva, Røros, © K.Glavatskiy

Spring examination

Course no.	Course title (credits)	Lectures and exercise coordinators	Candidates /Passed
RFEL1001	Natural Science and World Views (7,5)	Reidar Edvald Stølevik Annette Lykknes	54/44
KJ1020	Organic Chemistry (15)	Vassilia Partali	134/101
KJ1042	Basic Thermodynamics with Laboratory (7,5)	Signe Kjelstrup	85/58
KJ2022	Spectroscopic Methods in Organic Chemistry (7,5)	Nebojsa Simic	23/20
KJ2031	Inorganic Chemistry, Advanced Course	Karina Mathisen	7/7
KJ2044	Physical Methods in Structural Chemistry (7,5)	Stian Forselv	1/1
KJ2051	Analytical Chemistry, Advanced Course (7,5)	Øyvind Mikkelsen Florinel Gabriel Banica	15/15
KJ2053	Chromatography (7,5)	Rudolf Schmid	29/27
KJ2070	Environmental Chemistry (15)	Torunn Berg Trond Peder Flaten	23/17
KJ2071	Environmental Chemistry, Introductory Course (7,5)	Torunn Berg	24/24
KJ2095	Experts in Teamwork - Environmental Influences on Human Health (7,5)	Trond Peder Flaten	15/15
KJ3000	Organic Medicinal and Pharamaceutical Chemistry (7,5)	Derek James Chadwick	16/13
KJ8056	Chemical Sensors and Biosensors (7,5)	Florinel Gabriel Banica	1/1
KJ8100	Organic Medicinal and Pharamaceutical Chemistry (7,5)	Derek James Chadwick	6/6
KJ8105	Organometallic Compounds in Organic Synthesis (7,5)	Odd Reidar Gautun	1/1
TKJ4111	Organic Chemistry, Advanced Course (7,5)	Bård Helge Hoff	22/19
TKJ4130	Organic Synthesis, Laboratory (7,5)	Odd Reidar Gautun Bård Helge Hoff	7/7
TKJ4135	Organic Synthesis, Advanced Course (7,5)	Anne Fiksdahl	9/3
TKJ4170	Quantum Chemistry (7,5)	Henrik Koch	4/4
TKJ4175	Chemometrics(7,5)	Bjørn Kåre Alsberg	9/7
TKJ4190	Physical Chemistry, Project Work	Bjørn Kåre Alsberg	2/2
TKJ4215	Statistical Thermodynamics in Chemistry and Biology (7,5)	Per-Olof Åstrand	32/27

Participants at "The 6th International Workshop of IWNET 2012" in Røros, canoeing down the river. © K.Glavatskiy

Autumn examination

Course no.	Course title (credits)	Lectures and exercise coordinators	Candidates /Passed
RFEL3093	Episodes from the history of science (7,5)	Annette Lykknes	8/8
KJ1000	General Chemistry (15)	Håvard Karoliussen Torbjørn Ljones	192/168
KJ1030	Inorganic Chemistry (15)	Karina Mathisen	56/55
KJ1041	Chemical Bond, Spectroscopy and Kinetics (7,5)	Eirik Hjertenæs	108/91
KJ2050	Analytical Chemistry, Basic Course (7,5)	Øyvind Mikkelsen Florinel Gabriel Banica	-/-
KJ3022	Spectroscopic Methods in Organic Chemistry, Advanced Course (7,5)	Nebojsa Simic	16/14
KJ3050	Marine Organic Environmental Chemistry (7,5)	Øyvind Mikkelsen	12/12
KJ3053	Analytical Methods for Industrial- and Environmental Monitoring (7,5)	Øyvind Mikkelsen	9/8
KJ3059	Chromatography, Advanced Course	Rudolf Schmid	3/3
KJ3071	Applied Geochemistry (7,5)	Rolf Tore Ottesen	29/29
KJ3072	Advanced Aquatic Chemistry (7,5)	Trond Peder Flaten	17/15
KJ8053	Analytical Methods for Industrial- and Environmental Monitoring (7,5)	Øyvind Mikkelsen	1/1
KJ8056	Chemical Sensors and Biosensors (7,5)	Florinel Gabriel Banica	4/4
KJ8059	Chromatography, Advanced Course (7,5)	Rudolf Schmid	2/2
KJ8107	New Concepts in Organic Synthesis (7,5)	Bård Helge Hoff	3/3
KJ8902	Molecular Modelling (7,5)	Per-Olof Åstrand	5/5
KJ8903	Irreversible Thermodynamics (7,5)	Kirill Glavatskiy	1/1
TKJ4102	Basic Organic Chemistry	Odd Reidar Gautun	104/91
TKJ4180	Physical Organic Chemistry (7,5)		-/-
TKJ4200	Irreversible Thermodynamics (7,5)	Kirill Glavatskiy	9/9
TKJ4205	Molecular Modelling (7,5)	Per-Olof Åstrand	16/16
TKJ4510	Physical Chemistry, Specialization Project (15)	Bjørn Kåre Alsberg	3/3
TKJ4520	Organic Chemistry, Specialization Project (15)	Odd Reidar Gautun	-/-
TKJ4525	Organic Chemistry, Specialization Course (7,5)	Anne Fiksdahl	9/9

Re-sit examination

Course no.	Course title (credits)	Candidates/Passed
RFEL1001	Natural Science and World Views (7,5)	1/0
KJ1000	General Chemistry (15)	10/9
KJ1020	Organic Chemistry (15)	10/5
KJ1030	Inorganic Chemistry (15)	1/1
KJ1041	Chemical Bond Theory and Spectroscopy (7,5)	6/3
KJ1042	Basic Thermodynamics with Laboratory (7,5)	12/8
KJ2022	Spectroscopic Methods in Organic Chemistry (7,5)	2/2
KJ2031	Inorganic Chemistry, Advanced Course (7,5)	1/1
KJ2050	Analytical Chemistry, Basic Course (7,5)	2/1
KJ2051	Analytical Chemistry, Advanced Course (7,5)	1/1
KJ2053	Chromatography (7,5)	1/1
KJ2070	Environmental Chemistry (15)	3/3
KJ3000	Organic Medicinal and Pharamaceutical Chemistry (7,5)	3/2
KJ3021	Nuclear Magnetic Resonance Spectroscopy (7,5)	2/1
KJ3070	Advanced Aquatic Chemistry (15)	1/1
RFEL3093	Episodes from the history of science (7,5)	2/2
KJ8901	Enzyme Chemistry (7,5)	1/1
TKJ4102	Basic Organic Chemistry(7,5)	5/5
TKJ4111	Organic Chemistry, Advanced Course (7,5)	2/2
TKJ4135	Organic Synthesis, Advanced Course (7,5)	4/1
TKJ4180	Physical Organic Chemistry (7,5)	1/1
TKJ4215	Statistical Thermodynamics in Chemistry and Biology (7,5)	4/4

View from the old mining town Røros. © K.Glavatskiy

Technology students

3. year (MTKJ)
Asplin, Alexander
Bekkevard, Pål Unnerud
Borander, Venke
Buene, Audun Formo
Falck, Merete
Glasø, Martine Utland
Hansen, Ole Kudsk
Henriksen, Silje
Haarseth, Pia Kristine
Landsem, Elise
Nguyen, Phuong Toan
Ringheim, Ingvild

4. year (MTKJ)
Lund, Ingvild Teigen
Moen, Ingri Ullestad
Skjelbred, Kristin Marie
Skreddernes, Vilhelm

5. year (MTKJ)
Glansberg, Karin Märta
Hauge, Hans Henrik R.
Hogsnes, Morten Christian
Holden, Mia Cathrine Hellandsjø
Johansen, Maren Teresa
Kolstad, Aleksander
Myhre, Rolf Heilemann
Rydså, Line
Skjønsfjell, Ellen Martine
Solemslie, Henrik Winther
Tveeikrem, Marit Elise Endresen

Master students in progress

Chemistry (MKJ)
Aaen, Ingrid
Aakre, Iselin
Bakka, Thomas Aleksander
Berge, May Britt
Blomli, Janne Yttermo
Borkowska, Zuzanna
Finstad, Martin
Gjesteland, Ingrid
Haugen, Ingrid Naterstad
Hirkjølen, Morten
Jakobsen, Trygve Dagsloth
Johansen, Frank Edvardsen
Karlsen, Silje Sæther
Kirkemo, Fredrik Nestande
Kirste, Karsten Granlund
Lien, Vegard Torp
Linde, Henrik
Lindgjerdet, Per Magnus
Madland, Eva
Mikalsen, Ragni Fjellgaard
Nesbakken, Mari
Næss, Isabel Stubberud
Ofstad, Benedicte
Ophaug, Camilla
Pettersen, Iselin Esp
Simensen, Jan Tore
Slotten, Geir Andreas
Strand, Robin Viktor
Sylte, Kent-Ove Kragseth
Tveit, Marie Fossvoll
Van der Wijst, Cornelis Gerardus
Yttervik, Johan Hatling

Environmental toxicology and chemistry (MSENVITOX)
Hansen, Ailin Falkmo
Ramzan, Muhammad
Rusti, Elise Hermo
Vike, Kristine

Master of Science Education (MLREAL)
Baardsgaard, Margrete Marine
Grøndal, Stine Skimmeland
Horgheim, Jorunn Bårdsnes
Klungvik, Elina
Krongborg, Anne Ingelill Engvik
Marthinussen, Ingvild
Sandstad, Vidar
Skaret, Lise Bjerkestad
Solli, Cathrine Malvik

The following Ph.d. projects are in progress

PhD-student	Working title	Supervisors
Badina, Aderonke	Efficient production of fuels from biomass The use of microwave and hydrolic enzymes in processing of biomass.	Hoff, Bård Helge
Bugge, Steffen	Heteroaromatic compounds as new anticancer agents, diagnostic tools, and protozoal agents.	Hoff, Bård Helge
Bøyesen, Katrine	Combined Raman, X-ray Absorption, Scattering and diffraction studies on nanoparticulate VOx species in micro and mesoporous systems for the selective oxidation of propene and propane.	Mathisen, Karina
Catelli, Emilio	Norwegian cultural heritage: A chemical perspective	Banica, Florinel (main) Kvittingen, Lise
Davari, Nazanin	Molecular modeling of breakdown processesin electrically insulating liquids.	Åstrand, Per-Olof (main) Ingebrigtsen, Stian
Forselv, Stian	Catalytic conversion of 2nd generation biomass to liquid fuels over nanostructured hierarcial solids.	Mathisen, Karina (main) Svelle, Stian Bjørgen, Morten
Gebremariam, Kidane Fanta	Analytical methods for art objects investigation.	Kvittingen, Lise (main)
Gerontas, Apostolos	A history of the development of column chromatography: From Tswet to HPLC.	Lykknes, Annette (main) Hentschel, Klaus
Hjertenæs, Eirik	Quantum chemical calculations on sodium-graphite systems and development of a computional method utilizing non-orthogonal Slater determinants.	Koch, Henrik (main) Andersson, Stefan
Iftekhar, Shafia	Trace metals and natural organic matters in rivers	Berg, Torunn (main) Flaten, Trond Peder Mikkelsen, Øyvind
Karlsen, Morten	Synthesis of 13C-labelled standards for analysis of narcotics.	Hoff, Bård Helge (main) Liu, Hui-Ling
Kaspersen, Svein Jacob	New pyrrolo, thieno and furopyrimidine targeting tyrosine kinases (cancer) and protozoas: Synthesis and bioactivity.	Hoff, Bård Helge
Kristiansen, Tina	Aerogels: A new class of materials for catalytic purposes.	Mathisen, Karina (main) Nicholson, David G.
Kumelj, Tjasa	Free energy calculations of ligand-protein interactions.	Åstrand, Per-Olof (main
Løkken, Torbjørn Vegard	Analyser av vannduggpunkt og hydro-karbonduggpunkt i naturgass. (Determination of water dewpoint and hydrocarbon dew-point in natural gas.)	Schmid, Rudolf (main) Fredheim, Arne Olav
Mahmoodinia, Mehdi	Molecular modelling of the Fischer-Tropsch process.	Åstrand, Per-Olof (main) Chen, De
Martinsen, Morten	Development of an on-line monitoring platformand procedure for rapid environmental and processmonitoring of heavy oil extraction operations and industrial activity.	Mikkelsen, Øyvind (main) Schmid, Rudolf
Melnes, Silje	Rational drug design synthesis of potential selective inhibitors of tyrosin kinase 2.	Gautun, Odd Reidar
Nordløkken, Marit	Trace of elements in Norwegian deer.	Berg, Torunn (main superv.) Flaten, Trond Peder Steinnes, Eiliv
Raju, Rajesh	Optically active amphiphiles and artificial cells.	Gautun, Odd Reidar
Saepurahman	Spectroscopic studies of zeolites and zeolite facilitated oxygenate/hydrocarbon conversion reactions.	Mathisen, Karina (main superv.) Svelle, Stian
Sandbakk, Katrine Dretvik	Reverse electrodialysis - DC power from mixing of sea and river water.	Kjelstrup, Signe (main superv.) Burheim, Odne

PhD-student	Working title	Supervisors
Simic, Anica	Trace elements and persistent organic pollutants (POPs) in blood serum samples from the Nord-Trøndelag health study (HUNT) and the possible role of trace elements in type 2 diabetes.	Flaten, Trond P. (main superv.) Midthjell, Kristian
Skorpa, Ragnhild	A thermodynamic base for reaction kinetics. Studied by non-equilibrium molecular dynamics simulations.	Kjelstrup, Signe
Syed, Majid Bukhari	Isolation and structure elucidation of natural Bioactive molecules of plant origin.	Simic, Nebojsa
Takla, Marit	Methods to utilize waste heat in the ferro alloy industry.	Kjelstrup, Signe (main superv.) Burheim, Odne Kolbeinsen, Leiv
Tesfamariam, Gebrekidan M.	Enhancing the quality and relevance of chemistry teacher training education in Ethiopia: A study of the use and impact of small-scale, low cost experiments at Mekelle University.	Lykknes, Annette (main superv.) Kvittingen, Lise
Thvedt, Thor Håkon Krane	Enzymatic resolution coupled with in-situ racemisation for production of enantiopure amines. Application of the building blocks in preparation of potential antifungal compounds.	Hoff, Bård Helge (main superv.) Sundby, Eirik
Zaidi, Asma	Synthesis of highly unsaturated amino acids.	Partali, Vassilia (main superv.) Sliwka, Richard
Voldsund, Mari	Entropy production in process equipment.	Kjelstrup, Signe (main superv.) Ertesvåg, Ivar
Weggeberg, Hanne	Metal characterization of different size fractions. of airborne particulate matter and adverse health effects in humans.	Flaten, Trond P. (main superv.) Hilt, Bjørn
Wilhelmsen, Øivind	Non-equilibrium thermodynamics of phase transitions.	Kjelstrup, Signe (main superv.) Bedeaux, Dick
Waage, Magnus	Kinetic properties of gas hydrates	Kjelstrup, Signe (main superv.) van Erp, Titus

MSc in Chemistry

Aakre, Eva Kristin	**Forurenset sjøbunn – En vurdering av miljøundersøkelser som beslutningsgrunnlag for og dokumentasjon av tiltak i norske havner og fjorder**
Supervisors:	Professor Trond Peder Flaten Professor II Rolf Tore Ottesen
Examiners:	Research Scientist, PhD. Henning Keiding Bjerregår Jensen, NGU Professor Øyvind Mikkelsen
Egeness, Mari Jystad	**Comprehensive Two-dimensional Gas Chromatography: method development and verification by characterisation of petroleum fractions**
Supervisors:	Associate Professor Rudolf Schmid Principal Researcher Bente Seljestokken, Statoil Principal Researcher Anne Hoff, Statoil
Examiners:	Associate Professor , Dr. Scient Eirik Sundby, HiST Professor Anne Fiksdahl
Haugland, Marius Myreng	**Synthesis of a Novel Tocopherol/Carotenoid Derivative**
Supervisors:	Professor Vassilia Partali Richard Sliwka
Examiners:	Associate Professor Birte J. Sjursnes, HiØ Professor Emeritus/Dr.tech. Eva H. Mørkved
Henriksen, Stine	**Kartlegging og kjemisk karakterisering av oljeforurensning langs Trøndelagskysten**
Supervisors:	Associate Professor Rudolf Schmid Senior Researcher/PhD. Per Johan Brandvik, SINTEF Materials and Chemistry Senior Researcher/PhD. Liv-Guri Faksness, SINTEF Materials and Chemistry
Examiners:	Senior Reseacher/Dr.rer.nat Roland Kallenborn, NILU Professor Bjørn Kåre Alsberg
Hoholm, Rebekka Stavrum	**Synthesis and Characterization of Gold and Copper Nanoparticles in Mesoporous Frameworks**
Supervisors:	Associate Professor Karina Mathisen Professor Morten Bjørgen
Examiners:	Reseacher/PhD. Camilla Nordhei, IFE Professor Emeritus Reidar Stølevik
Høiås, Morten Juul	**Asymmetrisk katalytisk hydrogenering av enamider/enaminer for fremstilling av substituerte 2-aimnotetraliner**
Supervisor:	Associate Professor Odd Reidar gautun
Examiners:	Associate Professor Tore Lejon, UiT Associate Professor Bård Helge Hoff
Isaksen, Marte Eik	**Kartlegging og evaluering av miljøstatus i vannforekomster nær Statoils sandoljeprosjekt i Leismer (Alberta, Canada). Videreutvikling og uttesting av en ny type passiv prøvetaker for metaller i naturlig vann.**
Supervisors:	Professor Øyvind Mikkelsen Principal Reseacher Christian Collin-Hansen, Statoil
Examiners:	Professor Emeritus Knut Schrøder Associate Professor Rudolf Schmid
Larsen, Katrine Hervik	**Investigation on the Experimental Determination of Crude Oil in the Faeces from the Marine Copepod Calanus finmarchicus**
Supervisors:	Associate Professor Rudolf Schmid Researcher Anders J. Olsen, IBI Senior Reseacher Andrew Booth, SINTEF Materials and Chemistry Senior Researcher Alf G. Melbye, SINTEF Materials and Chemistry
Examiners:	Associate Professor Birte J. Sjursnes, HiØ Associate Professor Florinel G. Banica

Moen, Ingvill Marie	**Fraksjonering av atmosfærisk kvikksølv på Zeppelin, Ny-Ålesund**
Supervisor:	Professor Torunn Berg
Examiners:	Researcher Katrine Aspmo Pfaffhuber, NILU
	Professor Trond Peder Flaten
Noreng, Mona Skagseth	**Kjemisk karakterisering av oljeforurensninger i 14 år etter et eksperimentelt oljesøl på en strandsone i Arktis**
Supervisors:	Associate Professor Rudolf Schmid
	Senior Researcher/PhD. Liv-Guri Faksness, SINTEF Materials and Chemistry
	Senior Researcher/PhD Svein Ramstad, SINTEF Materials and Chemistry
Examiners:	Associate Professor Birte J. Sjursnes, HiØ
	Professor Øyvind Mikkelsen
Opsahl, Anette	**Characterization of Gold and Copper Species in Nanoporous Materials**
Supervisors:	Associate Professor Karina Mathisen
	Professor Morten Bjørgen
Examiners:	Reseacher/PhD. Camilla Nordhei, IFE
	Professor Magnus Rønning, IKP
Sørensen, Lisbet	**Parameters Governing the Adsorption of Crude and Bunker Fuel Oils to Seawater Suspended Particulate Matter**
Supervisors:	Associate Professor Rudolf Schmid
	Senior Reseacher Andrew Booth, SINTEF Materials and Chemistry
	Senior Researcher Alf G. Melbye, SINTEF Materials and Chemistry
Examiners:	Associate Professor Birte J. Sjursnes, HiØ
	Associate Professor Florinel G. Banica
Toftaker, Astrid	**Molbegrepet i kjemi**
Supervisor:	Associate Professor Annette Lykknes
Examiners:	Associate Professor Vivi Rignes, UiO
	Professor Lise Kvittingen

MSc in Chemistry/Technology

Blakstad, Guro	**Vinyl Amide Reactions in the Presence of Gold(I) Catalyst**
Supervisor:	Professor Anne Fiksdahl
Examiners:	Associate professor Tore Lejon, UiT
	Professor Anne Fiksdahl
Bøe, Maren Seljenes	**Organosolv pretreatment of biomass for biofuel and biorefinery applications**
Supervisors:	Associate Professor Bård Helge Hoff
	Reseacher Ingvild Andersen Johnsen, PFI
Examiners:	Senior Reseacher Kai Toven, PFI
	Associate Professor Bård Helge Hoff
Ellila, Georg	**Capillary forces and osmotic gradients in salt water – oil systems**
Supervisor:	Professor Signe Kjelstrup
Examiners:	Dr.ing Magnar Ottøy, Statoil
	Professor Signe Kjelstrup
Elnan, Jørund	**Screening of Inhibitors for Amine Degradation**
Supervisors:	Associate Professor Bård Helge Hoff
	Professor Hallvard Svendsen, IKP
	PhD Candidate Solrund Johanne Vevelstad
Examiners:	Senior Scientist Karl Anders Hoff, SINTEF Materials and Chemistry
	Professor Bård Helge Hoff
Gulbrandsen, Tore Aarhus	**Hot-water Extraction of Hemicelluloses by Microwave Heating**
Supervisors:	Associate Professor Bård Helge Hoff
	Professor Øyvind W. Gregersen, IKP
	Reseacher/PhD Ingvild Andersen Johnsen, PFI
	Researcher/PhD Mihaela Tanase Opedal, PFI
Examiners:	Senior Reseacher Kai Toven, PFI
	Associate Professor Bård Helge Hoff

Han, Jin	**Kobling av kirale fluorerte og ikke-fluorerte alkoholer til aromatiske heterosykler**
Supervisor:	Associate Professor Bård Helge Hoff
Examiners:	Director New Product Development/Cand.real. Reinert Fure, Borregaard AS
	Associate Professor Bård Helge Hoff
Isaksen, Stian Moe	**Isolation and Structure Elucidation of Bioactive Compounds from Plant Extracts**
Supervisor:	Associate Professor Nebojsa Simic
Examiners:	Associate Professor/Dr.ing Kåre B. Jørgensen, UiS
	Associate Professor Nebojsa Simic
Kaur, Maya Rajinder	**Gold(I) Catalyzed Tandem Cyclization Reactions**
Supervisor:	Professor Anne Fiksdahl
Examiners:	Associate Professor Tore Lejon, UiT
	Professor Anne Fiksdahl
Larsen, Synne	**Nukleofil aromatisk substitusjon på aromatiske heterosykler**
Supervisor:	Associate Professor Bård Helge Hoff
Examiners:	Dr.ing. Harald Svensen, Epax
	Associate Professor Bård Helge Hoff
Surdal, Cecilie	**Potential Inhibitors of Tyrosine Kinase 2: Synthesis of Important Intermediates**
Supervisor:	Associate Professor Odd Reidar Gautun
Examiners:	Associate Professor/Dr.ing Kåre B. Jørgensen, UiS
	Associate Professor Odd Reidar Gautun
Vo, Mong Truc	**Synthesis of a Precursor for a Carotenoid Cationic Lipid**
Supervisor:	Professor Vassilia Partali
Examiners:	Associate Professor Birte J. Sjursnes, HiØ
	Professor Vassilia Partali
Zefaniya, Papy	**Seebeck and Peltier coefficients of hydrogen electrodes related to the PEMFC**
Supervisors:	Professor Signe Kjelstrup
	Post.doc Odne Stokke Burheim
Examiners:	Senior Scientist Torleif Holt, SINTEF Petroleum Research
	Professor Signe Kjelstrup

MSc in Education, chemistry

Brekke, Elisabeth Raknes	**Undervisning av kjemisk binding som gir økt innsikt i stoffers oppbygning og egenskaper**
Supervisor:	Professor Lise Kvittingen
Examiners:	Associate Professor Vivi Rignes, UiO
	Professor Lise Kvittingen
Børset, Beate	**Studie av metaller i sedimentprofiler i området indre Trondheimsfjord**
Supervisors:	Professor Øyvind Mikkelsen
	Professor Trond Peder Flaten
Examiners:	Professor Emeritus Knut Schrøder
	Professor Øyvind Mikkelsen
Eidem, Bjørn	**Spredning av forurensning fra land til havnebasseng i Stavanger havn**
Supervisors:	Professor Trond Peder Flaten
	Professor II Rolf Tore Ottesen, NGU
Examiners:	Researcher Ola Anfin Eggen, NGU
	Professor Trond Peder Flaten

Elgaaen, Christian	**Undersøkelser om anvendbarheten av membranintroduksjons-massespektrometri (MIMS) for analyser av aminer i luft og vann**
Supervisor:	Associate Professor Rudolf Schmid
Examiners:	Dr.Scient Kolbjørn Zahlsen, SINTEF Materials and Chemistry
	Associate Professor Rudolf Schmid
Kongsvik, Marita Kjøsnes	**Geokjemisk kartlegging av overflatejord i Kristiansand**
Supervisors:	Professor Trond Peder Flaten
	Professor II Rolf Tore Ottesen
Examiners:	Researcher Tor Erik Finne, NGU
	Professor Trond Peder Flaten
Pettersen, Ann-Mari	**Geokjemisk kartlegging av overflatejord i Sandnes og Stavanger**
Supervisors:	Professor Trond Peder Flaten
	Professor II Rolf Tore Ottesen
Examiners:	Researcher Tor Erik Finne, NGU
	Professor Trond Peder Flaten
Særsland, Anne Lene	**Lære ved å gjøre, lære ved å skrive?**
Supervisor:	Associate Professor Annette Lykknes
Examiners:	Associate Professor Vivi Rignes, UiO
	Postdoc. Per Odd Eggen, PLU

MSc in Environmental toxicology and chemistry (MSENVITOX)

Hunnestad, Annie Vera	**The Effects of Macronutrient Enrichments (ammonium) on the Distribution of Four Bioactive Tracel Metals (Cd, Mo, Ni, Cu) in Seawater and Planktonic Biomass**
Supervisors:	Professor Trond Peder Flaten
	Associate Professor Murat Van Ardelan
Examiners:	Professor Emeritus Eiliv Steinnes
	Professor Egil Sakshaug, IBI
Nordum, Mats	**Metaller og naturlig organisk materiale i arktiske elver på Svalbard**
Supervisor:	Professor Torunn Berg
Examiners:	Researcher Katrine Aspmo Pfaffhuber, NILU
	Professor Trond Peder Flaten
Sanchez, Nicolas	**Distribution and Variation of the Trace Metal Iron in the Base of the Pelagic Marine Food Web: A Mesocosm Approach**
Supervisors:	Professor Trond Peder Flaten
	Associate Professor Murat Van Ardelan
Examiners:	Professor Emeritus Eiliv Steinnes
	Professor Egil Sakshaug, IBI
Trefjord, Terese	**Investigations on the Applicability on Membrane Introduction as a Sampling Technique for Oil in Air and Water with Flame Ionization Detector (FID) and Mass Spectrometry (MS) Detection**
Supervisors:	Associate Professor Rudolf Schmid
	PhD candidate Morten Martinsen
	Principal Reseacher Christian Collin-Hansen, Statoil
Examiners:	Dr.Scient Kolbjørn Zahlsen, SINTEF Materials and Chemistry
	Professor Torunn Berg

PhD in Chemistry, finished 2012:

Lervik, Anders	**Energy dissipation in biomolecular machines**
Trial lecture	Mathematical modeling of neural communications with specific attention to Hodgkin-Huxley theory (Nobel Prize in Physiology or Medicine 1963).
Main supervisor	Professor Signe Kjelstrup
Co-supervisor	Professor II Fernando Bresme
Evaluation Committee	Professor Hong Qian, Department of Applied Mathematics, University of Washington, USA Professor Poul Nissen, Århus University, Department of Molecular Biology and Genetics, PUMPKIN, Denmark. Associate Professor Titus van der Erp, Dept. of Chemistry, NTNU
Mohsin, Muhammad Ali	**Sulfur-metal Interactions with Applications in Electrochemical Sensors**
Trial lecture	Chemical Sensors Based on Mechanical Transduction
Supervisor	Associate Professor Florinel Gabriel Banica
Evaluation Committee	Professor Kurt Kalcher, Karl Franzens University of Graz, Austria Dr. Nicolae Spataru, Romanian Academy, Institute of Physical Chemistry, Romania Professor Torbjørn Ljones, Department of Chemistry, NTNU
Strand, Ragnhild Beate	**Preparation and Catalytic Application of imidazolium and triazolium salts as new Chiral N-Heterocyclic Carbene (NHC) precatalysts**
Trial lecture	Ring and Chain Tautomerism in Heterocylic Systems
Supervisor	Professor Anne Fiksdahl
Evaluation Committee	Professor Jan Bergmann, Karolinska Institutet, Sweden Professor Lise-Lotte Gundersen, Department of Chemistry, University of Oslo Associate Professor Odd Reidar Gautun, Department of Chemistry, NTNU
Muhammad Zeeshan	**Synthesis and properties of long chain polyenes – synthesis and properties of cationic and anionic polyene lipids**
Trial lecture	Synthesis and properties of natural and unnatural polyenes
Main supervisor	Professor Vassilia Partali
Co-supervisor	PhD Hans-Richard Sliwka
Evaluation Committee	Professor Dr Bernd Schaefer, Ruprecht-Karls-Universität in Heidelberg / BASF SE, Ludwigshafen, Germany Professor Dr Peter Molnar, University of Pécs Medical School Hungary Associate Professor Nebojsa Simic, Department of Chemistry, NTNU

"Hyttklokka". The bell was used to notify workers at the smelter hut when work started and finished. © K.Glavatskiy

Student Exchange from NTNU, Department of Chemistry

Name	Specialization	Level	Institution
Bakka, Thomas A.	MKJ-Org.chem	MSc, 4th yr	University of Berkeley, USA
Dolva, Amund	MTKJ-Org.chem	MSc, 5th yr	ETH, Switzerland
Glansberg, Karin M.	MTKJ-Org.chem	MSc, 4th yr	ETH, Switzerland
Hauge, Hans Henrik	MTKJ-Phys.chem	MSc, 4th yr	TUM, Germany
Hogsnes, Morten	MTKJ-Org.chem	MSc, 4th yr	TUM, Germany
Mikalsen, Ragni F.	MKJ-Struc.chem	MSc, 4th yr	ETH, Switzerland
Myhre, Rolf H.	MTKJ-Phys.chem	MSc, 5th yr	University of Valencia, Spain
Rydså, Line	MTKJ-Org.chem	MSc, 4th yr	Uppsala University, Sweden

Student exchange to NTNU, Department of Chemistry

Name	Institution
Barbarin Abarzuza, Iranzu	Univ. of Basque Country, San Sebastián, Spain
Bagnoli, Luigi	Politecnico di Torino, Italy
Bellings, Lotte	Katholieke Universiteit Leuven, Belgium
Bergier, Mohena	University Paul Sabatier, Toulouse, France
Blijleven, Esther	Hogeschool Leiden, Netherlands
De Winter, Giel	Katholieke Universiteit Leuven, Belgium
Druel, Florian Jean Daniel	University of Rouen, France
Duricova, Ivana	Technical University in Zvolen, Slovakia
Fleischer, Timo	Christian-Albrechts-Universität zu Kiel, Germany
Gan, Shye Fern	Nanyang Technological University, Singapore
Grandl, Markus	Technische Universität München, Germany
Gschwend, Dominic Michael	ETH Zürich, Switzerland
Hansen, Christine	Georg August University Göttingen, Germany
Izaguirre Bracamonte, Luis C.	Universidad Central de Venezuela, Caracas
Jordan, Aline Maria	Germany
Kaneta, Yusuke	Tokyo Institute of Technology, Japan
Karlsson, Julia S.	Uppsala Universitet, Sweden
Landin, Alyssa	Luther College, Decorah, Iowa, USA
Lange, Sandra	Georg-August-Universität Göttingen, Germany
Lavagnini, Ennio	Universita degli studi di Padova, Italia
Lee, Saemi	Pukyong National University, Korea
Madziara, Nina	University of Lodz, Poland
Mauhart, Johannes	Graz University of Technology, Austria
Neirinck, Nelson J.	University of Gent, Belgium
Osborne, Chan Ao Bang	Nanyang Technological University, Singapore
Petreikyte, Indre	Vilnius University, Lithuania
Pilz, Irene C.	TU Bergakademie Freiberg, Germany
Piskor, Mateusz Z.	University of Hamburg, Germany
Poh, Audrey	Nanyang Technological University, Singapore
Rodriguez Larrañaga, Mikel	University of Basque Country, Spania
Smolders, Simon Jan	Katholieke Universiteit Leuven, Belgium
Stassin, Timothée Marie	Katholieke Universiteit Leuven, Belgium
Tyoh Whei Theng, Michelle	Nanyang Technological University, Singapore
Van Den Bergh, Matthias	Katholieke Universiteit Leuven, Belgium
Woh, Joanne	Nanyang Technological University, Singapore
Wong, Xin Yee	Nanyang Technological University, Singapore
Zolubas, Giedrius	Vilnius University, Lithuania

Academic Staff

Organic Chemistry

Group Leader
Associate Professor, Dr.Scient
Bård Helge Hoff

Associate Professor, Dr.ing.
Odd Reidar Gautun

Professor, Dr.rer.nat. (Fribourg). Vassilia Partali

Professor, Dr.ing.
Anne Fiksdahl

Associate Professor, Dr.Scient.
Elisabeth Egholm Jacobsen

Associate Professor, Ph.D. (Niš), Nebojsa Simic

Applied Theoretical Chemistry

Group Leader
Professor, Dr.scient.
Bjørn Alsberg

Professor, Dr.techn.
Signe Kjelstrup

Professor, Ph.D. (Lund)
Per-Olof Åstrand

Adjunct Professor
Fernando Bresme

Professor, Ph.D. (Århus).
Henrik Koch

Professor, Ph.D.
Torbjørn Ljones

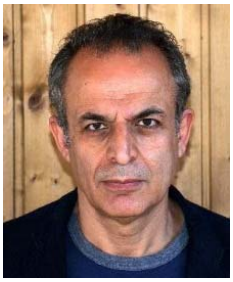
Associate Professor, PhD
(Amsterdam)
Titus Sebastiaan van Erp

Environmental and Analytical Chemistry


Group Leader
Professor, Dr.Scient
Øyvind Mikkelsen


Adjunct professor
Per Johan Brandvik


Associate Professor, Ph.D.
Karina Mathisen


Associate Professor,Dr.Scient
Murat V. Ardelan


Professor, Dr.ing.
Trond Peder Flaten


Professor, Ph.D. (London)
David Nicholson


Associate Professor, Dr.ing.
Florinel G. Banica


Professor, Dr.Scient.
Lise Kvittingen


Adjunct Professor
Rolf Tore Ottesen


Professor, Dr.scient.
Torunn Berg


Associate Professor, Ph.D.,
Annette Lykknes


Associate Professor, Dr.rer.nat.
(Zürich). Rudolf Schmid

Administrative staff


Head of department
Marie-Laure Olivier


Administrative manager
(- May2012)
Lena Frostad


Administrative manager
(July 2012 -)
Gunhild Meistad


Executive officer
Thea Berg Fines


Higher Executive Office
Gerd Flataas


Higher executive officer
Ingrid Kristine Tømmerdal


Higher executive officer
Bjørn Syvertsen


Executive officer
Inger Marie Frøseth

Technical staff


Staff engineer
Stein Almo


Head engineer
Susana Villa Gonzalez


Senior engineer
Tron Rolfsen


Head engineer
Trine Naalsund Andreassen


Head engineer
Julie Jackson


Staff engineer
Gunnar Svare


Staff engineer
Julie Asmussen


Head engineer
Nina Klausen


Staff engineer
Roger Aarvik


Head engineer
Syverin Lierhagen

Student assistants

Augestad, Elias H.
Bakka, Thomas A.
Blomli, Janne
Borander, Venke
Brandvik, Trond
Buene, Audun F.
Bukhari, Syed Majid
Bø, Fredrik H.
Courtade, Gaston
Dalane, Kristin
Eraker, Øyvind J.
Falck, Merete
Fauskanger, Tine O.
Finstad, Anne
Flo, Jørgen
Hammersland, Kine
Haugen, Linn C.
Haugland, Marius Myreng
Holden, Mia C.H.
Iftekhar, Shafia
Jahrsengene, Gøril
Juell, Rosemary A.
Karlsen, Silje S.
Kirste, Karsten G.
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Guest professors/researchers/lecturers

Erik Krogh Applied Environmental Research Laboratories Department of Chemistry, Vancouver Island University	7. – 16.5.2012
David J. Newman Natural Product Branch, the National Cancer Institute, the National Institutes of Health, USA	19. – 20.3.2012
Marta Pokrzywnicka Faculty of Chemistry, University of Warsaw	5.11.2012 – 28.2.2013
Jean Marc Simon University of Bourgogne, Carnot Laboratory, Dijon	17. – 21.12.2012
Brigitte van Tiggelen Université catholique de Louvain	4. – 17.6.2012

A magic moment in the old mining town of Røros. © K.Glavatskiy

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