

Annual Report 2008

# Department of Chemistry

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### **COVER PAGE**

Associate Professor Morten Bjørgen just left his base at the peak of Karlskråtind in Romsdal.

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## The State of the Department of Chemistry 2008

**Introduction.**—In last year's report on the State of the Department, I wrote: "Paradoxically these are turbulent times for university funding despite a booming economy." How quickly the economic scene has changed from a situation in which economic experts proclaimed a cloudless economic sky to the current picture of global doom and gloom. We can only hope that the situation remains paradoxical but this time in our favour. Hopefully, there is motivation to increase research funding in the university sector from 2009 although according to our omniscient Faculty the forecast for 2009 is that we are in for a rougher ride than in 2008.

**Measures to increase income.**—Nevertheless, I am impressed with the activities and productivity of some of our researchers who are operating under very trying circumstances. There are bright points that should be emphasised. Bearing in mind that of the three chemically-related departments, the Department of Chemistry's main role is to take care of basic or curiosity-driven research we have a balanced strategy aimed at increasing external funding that is additional to attempts to acquire support from a cash-strapped Research Council. We have implemented measures to stimulate those activities that generate external income whilst balancing this against the requirement that the Department also carries out basic research. Unfortunately, this process is time consuming. The following example gives some idea of the time scale before a project can be implemented.

**An example.**—NTNU will soon sign a contract with StatoilHydro on collaboration projects. One of these, which concerns this department, is centred on analytical-environmental aspects connected to extracting oil from Canadian oilsand. The formalities included a visit by NTNU Rector Torbjørn Digernes to Canada to sign a Memorandum of Understanding with our partner Canadian University. This project arose out of a desire to find a niche with Statoil that we could fill. From the initial contact and discussions I had with StatoilHydro (Dr. Christian Collin Hansen) in 2005, the project has been refined and developed between us and StatoilHydro and we are now about to start. In addition to myself (as Project Leader), Øyvind Mikkelsen and Rudi Schmid (Principal Investigators) have enthusiastically played important roles in bringing the project to the contract stage.

**International Master Degree.**—In order to further develop the environmental collaboration with StatoilHydro we have embarked on a collaboration that also includes the Department of Biology and SINTEF. The result is an International Master Degree in Environmental Toxicology. Sterling work on this has been carried out by Øyvind Mikkelsen, Trond Peder Flaten and Torunn Berg.

**Industrially financed Professorship.**—In the course of negotiations with StatoilHydro I requested that the company consider the benefits to them of financing an adjunct professor position from 2009

at our department. The response was positive and we are working on a mutually acceptable definition of this position which we anticipate will be ready for implementation in 2009. This position will strengthen the aforementioned International Master Course.

**Centre of Advanced Studies.**—We are pleased that we were able to contribute to research at the Centre of Advanced Studies in Oslo by granting Professor Signe Kjelstrup leave of absence to work there as a Group Leader. Signe was able to fully concentrate on her research into Nature-inspired Chemical Process Design and achieved interesting results. Accompanying Signe were Professors Dick Bedeaux and Henrik Koch as vice Group Leader (who has a highlight in this report) and PhD students Isabella Inzoli and Kirill Glavatskiy.

**The Max IV Project.**—In April we organised a conference entitled "the Nordic-Baltic Synchrotron Research Initiative Kick-off Meeting" The two day meeting was held at Jægtvolden some two hours drive north of Trondheim. Representatives from all of the Nordic and Baltic countries attended. The meeting culminated in a unanimous declaration supporting the proposed Swedish Max IV synchrotron project and redefining it as a Nordic-Baltic project. The process further will hinge on intergovernmental contacts in 2009 and a good case from researchers in the different countries. The Norwegian case is being worked out and will be presented in early 2009. This department in partnership with the Department of Physics has the key role here. This project will be the most ambitious research collaboration ever carried out within the Nordic region.

**The Swiss-Norwegian Beamlines.**—The reason we organised this meeting is grounded on the department's many years activities within the Swiss Norwegian Beamlines (SNBL) at the European Radiation Facility in Grenoble (ESRF). Partly because this department (together with the Department of Physics) founded the SNBL Consortium, the administrative staff went on a study trip there in April. They found the facility rather an eye-opener because of its technical sophistication and efficient administration and returned much invigorated.

**Innovation.**—Another aspect of the department's strategy is to identify and bring forth projects that are innovatively promising. An innovative project in particular that stood out in 2008 is from the group led by Professor Vassilia Partali. Vassilia and her coworkers project concerns gene therapy delivery and has societal relevance.

*David G. Nicholson  
Head of Department*



## Bridging Chemistry and Art: The case of Ethiopian works of art

One of the disciplines where art and science meet is conservation science. In this field chemistry plays a great role in the technical examination and conservation of cultural heritage in general and of art objects in particular.

There are various areas where chemistry can be applied in conservation science. It is used in the determination of chemical composition of painting components such as pigments, extenders, binding media, and varnishes. Chemistry is instrumental in characterization of the artists' techniques employed during execution. Understanding of these materials and painting techniques help conservators to decide on the best approach for conservation and restoration of the artefacts. The material composition can also provide information about the age and origin of art objects, thereby establishing provenance and authenticity. Such technical examination is of great importance to art historians who are concerned with the where, when, why, and how questions of past events and artistic material sources related to the art works. The chemical composition of these objects exposed by scientific analysis gives them historical and cultural meanings.

The other application is in the study of causes for degradation of art objects, the resulting corrosion products, the mechanisms and kinetics associated with the deterioration processes. This greatly aids to plan best interventions to stop, or at least slow down, deterioration. Chemistry is also vital in assessing the effect of materials and methods used in the course of repairing, consolidation, restoration and conservation.

A variety of analytical techniques are used for technical studies of works of art. A paramount requirement for such techniques is that they should be non-invasive and non-destructive with respect to the valuable works of art as much as possible.



Fig. 1 Medieval wall painting in poor state of conservation, Korkor Mariam monastery, Tigray

Our research project entitled, the study of Ethiopian paintings and illuminated manuscripts from the chemical perspective, is concerned with the

technical examination of Ethiopian works of art using a combination of analytical techniques such as XRF, SEM-EDS, micro Raman, IR, XRD, and polarized light microscopy. Attempts will be made to trace the origin of some of the pigments used in the paintings. Changes in the chemical composition of the painting materials attributed to ageing, the impacts of environment and human activity will also be assessed. This pursuit of scientific investigation on artistic objects will contribute to the characterization and documentation of traditional materials, technologies, and knowledge in the production of the cultural heritage.



Fig 2. Mural from Narga Silassie monastery on Lake Tana



Fig 3. Old illuminated manuscript on vellum, Kibran Gabriel Monastery

At the end of 2008, a field work in Ethiopia was carried out. The main objectives were to visit some of the potential research sites, gather preliminary information and conduct analysis on the spot of paintings and illuminated manuscripts with a portable XRF spectrometer. A number of mural paintings, icons and manuscripts were analysed in churches and monasteries located in different parts of Tigray, Lalibela and its vicinity, Gondar and Lake Tana areas. Attempts were also made to work on few of the collections of three museums in Addis Ababa and Tigray region

Kidane F. Gebremariam, Lise Kvittingen and Florinel G.Banica

## Surface Electrochemistry of metal chalcogenides and their bio-organic derivatives

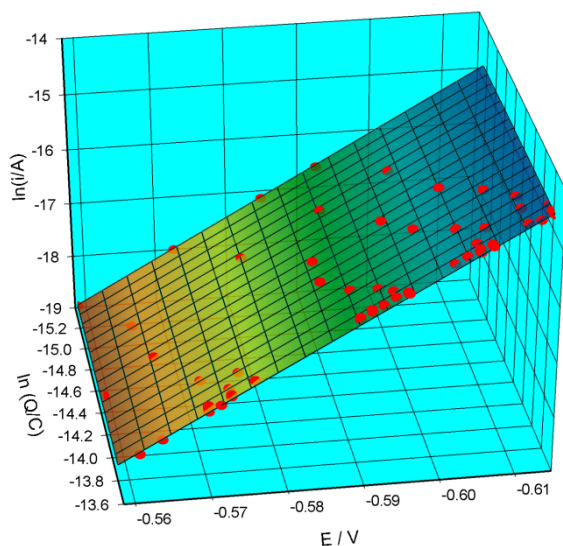
Chalcogenide is the collective name ascribed to the compounds of sulfur, selenium and tellurium. Metal chalcogenides are compounds of a great importance for natural environment, biological systems and industry. Thus, metal sulfides are well known raw material for production of a series of important metals. Besides, metal chalcogenides are of a particular relevance to marine chemistry. In this respect, recent research work in this field focuses on the occurrence and properties of metal sulfides as complex compounds or clusters. As a consequence of the extremely low solubility of metal sulfides, Environment Technology resorts to such compounds for removal of toxic metal pollutants. Some chalcogenides are also employed as advanced materials for nano-technology, chemical sensors, and semiconductors.

In addition to their particular role in the mineral world, chalcogens are also of a distinct importance in living organisms. Cysteine - an amino acid that contains the sulfhydryl group and is formally a hydrogen sulfide derivative - plays an outstanding role in protein structure and also can function as an anchor bridge for enzyme immobilization on metal surfaces. Cysteine residues may also bind to heavy metal ions ( $\text{Pb}^{2+}$ ,  $\text{Hg}^{2+}$ ) because of the high affinity between sulfide and the soft metals. This reaction can deform and inactivate the native protein, and is therefore involved in heavy metal poisoning. On the other hand, metallothionein - a cysteine rich protein - plays an active role in metal detoxification. This protein is involved in biological remediation of heavy metal pollution and is also employed as a biomarker for metal pollution. Metal-sulfur clusters occur as prosthetic groups in hydrogenases - a class of enzymes that catalyze the reduction of the hydrogen ion to molecular hydrogen and displays promising prospects for applications in hydrogen technology. Therefore, metal sulfide investigations allow modeling the active sites of some enzymes of environmental and technological significance.

- Our recent achievements in electrochemistry of chalcogenides can be summarized as follows:
- Electrochemical preparation and investigation of metal sulfides and thiolates as molecular or thin layers on metal surfaces [1, 2];
- Self-assembly of bio-compounds on metal surfaces using chalcogenide functions as binding groups [3-7];
- Application of piezoelectric nano-gravimetry for the investigation of surface layers including chalcogenide-based anchoring groups [5, 7];
- Investigation of metal ion interaction with sulfide ions ( $\text{S}^{2-}$  or  $\text{HS}^-$ ) at the concentration level characteristic for ocean water [8].

As a continuation of our previous work in this field, we intend to refine the theoretical approach recently outlined [1] in order to render it suitable for data processing by a multi-variable approach using advanced computer graphing and statistical treatment. Such an approach is more accurate and enlightening as compared to the standard single-variable method. As an example, the Figure displays a 3-dimensional plot and data fitting for the reduction of mercury sulfide in the form of surface layer on a mercury electrode. Data in this graph fits very well the equation of a plane and allow testing the validity of theory assumptions.

Further refinement of theoretical and experimental methods will allow determining important physico-chemical constants of chalcogenide ions, chalcogenide derivatives and their metal salts in natural media such as marine water and biological fluids.



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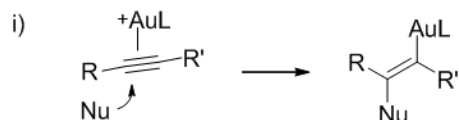
Florinel Banica



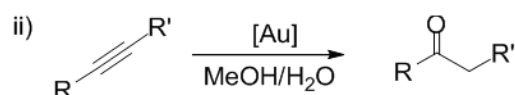
## NEW GOLD CATALYSED CYCLISATION REACTIONS

### Gold catalysis; background

Gold catalysis has been neglected by organic chemists for a long time. However, homogenous gold catalysis of organic reactions has in recent 5 years become a rapidly expanding field. Gold complexes are less oxophilic than other common Lewis acids, but they are highly reactive as carbon Lewis acids (e.g. double and triple bonds). Gold catalysts can therefore react in a very selective way and give access to highly complex molecules.



Gold complexes coordinate to C-C multiple bonds. Gold catalysts interact with the p-system and activates for nucleophilic attack (see i) below). Alkynes are successfully used as substrates for gold catalysis. Hydration reactions of alkynes to form the respective ketones are well known (ii):



### Cyclisation reactions of 1,6-diynes

Gold catalysed hydration of 1,6-diynes has previously not been studied.

The low yields, high temperature and often harsh acidic conditions previously applied for toxic mercury(II) or gold catalysed hydration of alkynes, encouraged us to investigate less vigorous

conditions for the hydration of 1,6-diynes catalysed by gold(I)-complexes.

We have developed new gold catalyzed cyclisation reactions for 1,6-diynes (1a-g, see I below).

### New gold catalyzed cyclisations of 1,6-diyne

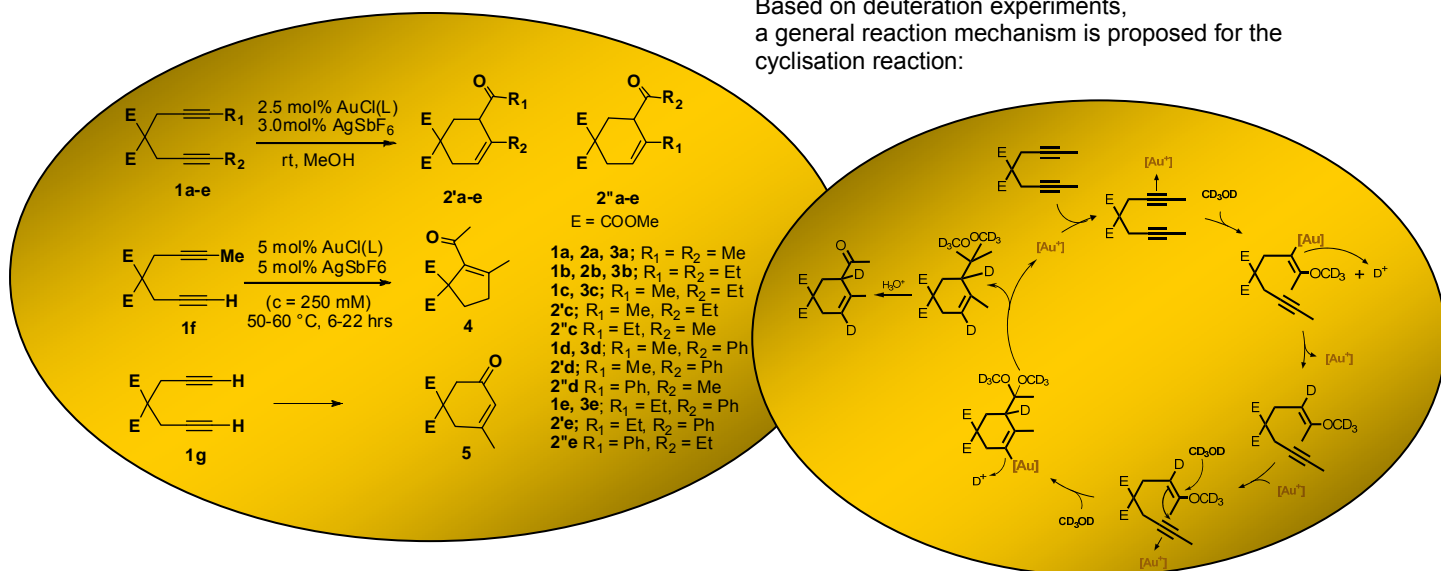
Symmetrically (1a,b) and unsymmetrically (1c-e) substituted 1,6-diynes underwent cyclisation reactions to afford cyclohexene derivatives 2a,e.

The mono-terminal diyne 1f and the di-terminal diyne 1g provided, respectively, cyclopentene and cyclohexenone derivative (4,5):

I:

### II: Mechanism:

Based on deuteration experiments, a general reaction mechanism is proposed for the cyclisation reaction:



Anne Fiksdahl

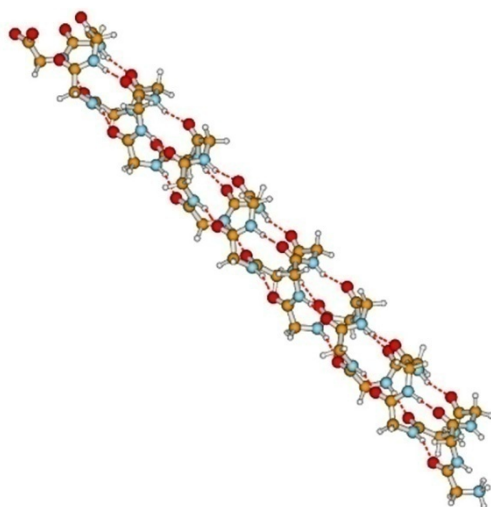
## The art of making quantum chemistry calculations faster

The field of quantum chemistry deals with the theoretical description of molecular systems at the atomic scale using computer simulations. From being a rather exotic area of chemistry 20 years ago, the methods of quantum chemistry are nowadays widely used in most areas of chemistry. This is due to two main driving factors: the advance of the electronic computer and the improvement of the theoretical formulations and implementations in computer programs.

The theoretical foundation of quantum chemistry is quantum mechanics and the central equation is the Schrödinger equation (1926)

$$H\Psi = \Psi E$$

where the wave function  $\Psi$  contains all information about the electronic structure of the electrons in the molecular system and  $E$  is the total energy. Only the Hamiltonian operator  $H$  is known and the equation must be solved to determine the wave function and total energy. The wave function is a complicated function of the position of all the electrons and



nuclei in the molecule. A solution of the Schrödinger equation amounts to determining the wave functions and even if we restrict our treatment to the

electronic structure for a fixed position of the nuclei this equation can only be solve analytically for one-electron. Thus approximations must be introduced and much research in quantum chemistry revolves around developing new and efficient approximations in this way obtaining new insight into the wave function. Over the years many methods have become standards in electronic structure calculations and these are the methods that are most widely used. One problem that remains unsolved for many models is the scaling of computational requirements with respect to the size of the system; ideally we would like this to be linear, such that a system of double size only requires twice the computational requirements. During the stay at CAS we have developed new algorithms for Coulomb and exchange energy contributions to the electronic energy. These methods are based on the Cholesky decomposition that is a very efficient way to remove redundant information in the calculations. The linear dependence in matrices are in this way removed and never need to be calculated explicitly, this together with a straightforward testing for zero's give the improvement. We have observed three orders of magnitude speedup compared to the standard methods. The algorithms and results are published in Ref. [1] and we refer the reader to this for more detailed information.

*Henrik Koch*

Reference:

Linus Boman, Henrik Koch and Alfredo Sanchez de Meras, J. Chem. Phys. 129, 13107 (2008).

## The Fluoro-organic group: Towards Greener Chemistry by Ruthenium Catalysed Asymmetric Transfer Hydrogenation (ATH)

### Background

We have recently reported the synthesis,<sup>1</sup> and later the asymmetric reduction,<sup>2</sup> of a series of  $\alpha$ -fluoroacetophenones using Corey's proline based catalyst (*R*)-MeCBS. High enantiomeric excess and yield were obtained. However, to develop catalytic and more environmental friendly processes asymmetric transfer hydrogenations (ATH) have now been investigated.

### Asymmetric transfer hydrogenation (ATH)

The catalysts were constructed from  $\text{RuCl}_2(\text{mesitylene})_2$  and  $[\text{RuCl}_2(\text{p-cymene})_2]$  complexed with chiral diamine ligands, (Figure 1).

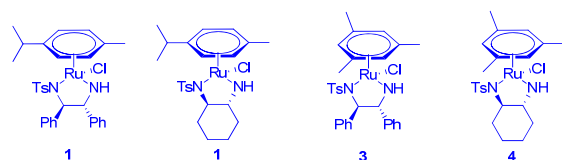
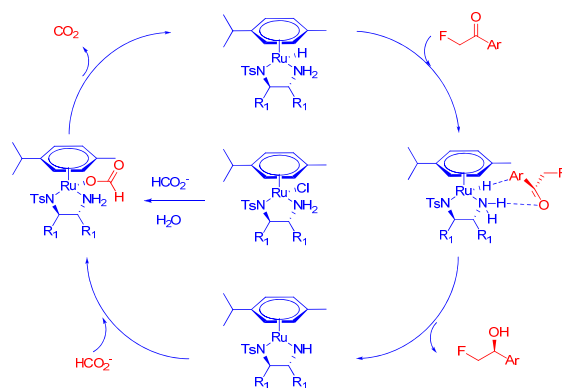


Figure 1. Catalysts used in the study.

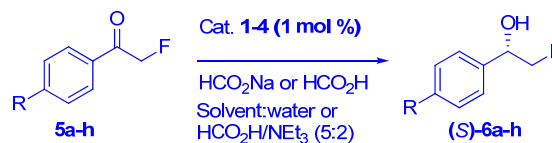
The benefits of these reduction systems are that cheap and safe reductive agents as *i*-PrOH and formic acid can be used. Moreover, reductions can be performed in water and also in the presence of air.<sup>3</sup> The proposed catalytic mechanism is shown in Scheme 1.



Scheme 1. Proposed catalytic mechanism for ATH (Xiao et al.)<sup>3</sup>

We decided on the use of formic acid as hydrogen donor and explored the ATH of eight different  $\alpha$ -fluoroacetophenones in both water and formic acid/triethylamine using catalyst 1-4 in 1 mol %, see Scheme 2.

The electronic content at the reacting carbonyl carbon was varied to identify possible electronic effects on the enantioselectivity and rate. Table 1 summarises the results using catalyst 3 in the two reaction medias.



Scheme 2. ATH of  $\alpha$ -fluoroacetophenones 5a-h.

Table 1. ATH of substrates 5a-h using catalyst 3 in water and formic acid/triethylamine

Substrate (R)	Water		HCO <sub>2</sub> H/NEt <sub>3</sub>	
	Conv. (h.)	ee (%)	Conv. (h.)	ee (%)
OMe 5a	>99 (5)	95.0	>99 (2)	96.0
OBn 5b	71 (20)	90.0	>99 (2)	97.5
H 5c	>99 (2)	95.5	>99 (2)	97.0
F 5d	>99 (5)	91.0	>99 (2)	93.5
Br 5e	>99 (5)	90.5	>99 (2)	91.0
CF <sub>3</sub> 5f	>99 (5)	96.0	>99 (2)	90.5
CN 5g	45 (20)	84.0	>99 (2)	88.0
NO <sub>2</sub> 5h	99 (20)	76.5	>99 (2)	84.5

The (*S*)-alcohols could be obtained in ee from 97.5 to 85.5. The selectivity was very dependant on both catalyst and substrate structure. The highest enantiomeric excess was obtained for substrates having electron donating substituents using catalyst 1 and 3 in formic acid/triethylamine. Only in reduction of substrate 5f was a higher selectivity observed in water.

Further, comparing the results with rates and selectivity in the acetophenone series, implies that the electronic content of the carbonyl carbon is of minor importance for enantioselection. This effect can rather be explained by other factors such as change in  $\pi$ - $\pi$  interactions, solvation effects or dispersion interactions.<sup>4</sup>

Bård Helge Hoff and Erik Fuglseth (Accepteded J. Fluorine Chem. 2009)

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## Muscular contraction and the calcium pump

As was shown by Huxley (1953), Huxley & Niedergerke (1954) and Huxley & Hanson (1954), the contraction of skeletal muscles is due to the sliding motion of myosin filaments along actin filaments. The interaction between the filaments is created by cross bridges extending from the myosin.

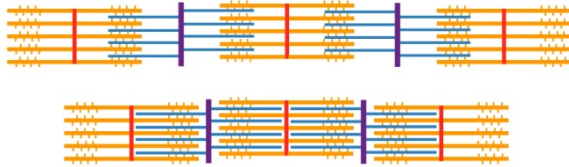


Fig. 1: The top figure is a relaxed muscle fibre and the bottom one a contracted muscle. The orange lines are myosin and the blue lines are actin molecules.

According to the theory by Huxley (1969), the heads of the filaments first attach to the actin and then undergo a conformational change whereby the angle of attachment is changed. This then causes a movement of the myosin along the actin. The energy for this process is derived from the hydrolysis of ATP to ADP and inorganic phosphate Pi. ATP binds to the myosin head and hydrolysis takes place. The calcium ions are stored in the sarcoplasmic reticulum, an organelle made for that purpose. When the nerve releases sodium and potassium ions, the surface of the reticulum depolarizes and the calcium ions are released into the sarcoplasm around the muscle fibers. The calcium then binds to the actin after which the myosin head also binds to the actin. The ADP and

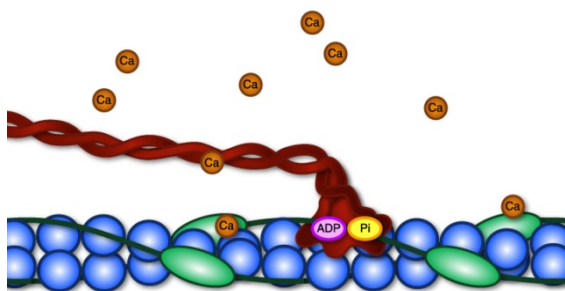


Fig. 2: After two calcium ions (brown) attach themselves to the actin, the myosin head also attaches itself to the actin molecule.

the Pi then detach from the myosin head which uses the energy for the conformational change to shorten the muscle fibre. When the muscle relaxes, Ca<sup>2+</sup>-ATPase pumps the calcium ion back to the reticulum, the myosin head detaches itself from the actin, and ATP binds to the myosin head.

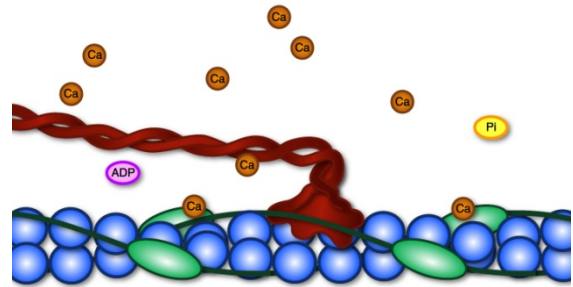


Fig. 3: After ADP (purple) and Pi (yellow) detach themselves the myosin head changes conformation and moves the actin relative to the myosin.

An important role in the whole process is played by the calcium pump, the Ca<sup>2+</sup>-ATPase (a protein), and we will mainly focus on the description of this pump using non-equilibrium thermodynamics. It is

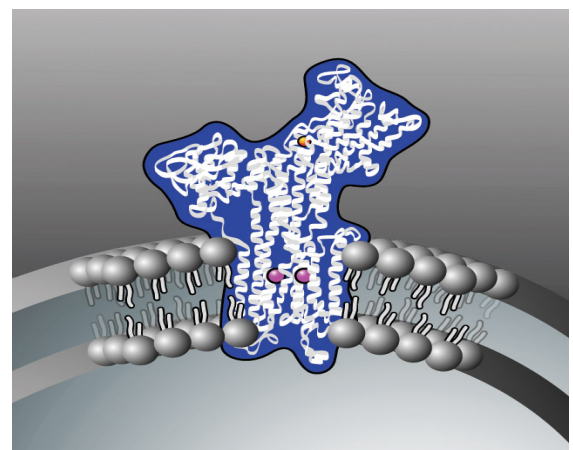


Fig. 4: The Ca-ATPase with 2 bound Ca ions in the lower part and 1 ATP molecule in the upper part .

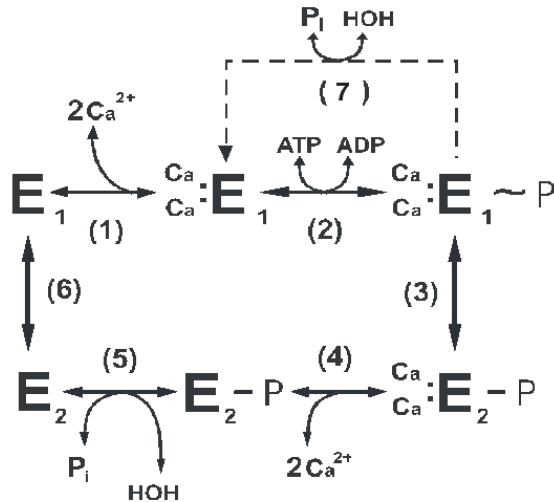


Fig. 5: The enzyme cycle.

common to describe how it works by a diagram of the enzyme cycle a so-called Post-Albers diagram, see Fig. 5. The protein has two configurations, E1 and E2. In the first state in the left top corner, the protein is in the E1 configuration and nothing is bound to it. In the first step, two calcium ions are bound inside the protein. In the second step, ATP is bound to the protein and splits into ADP, which goes back into the sarcoplasm, and organic phosphate, Pi, which binds to the protein. In the third step, the Pi changes location in the protein and the energy is used to modify the E1 configuration into an E2 configuration. In the fourth step in the cycle, the high energy of E2 allows calcium ions to go into the reticulum. In the fifth step, Pi unbinds. In the sixth step, the configuration changes back to E1. Depending on the thermodynamic forces involved, all these steps may be in the forward or in the backward direction. The process just described, is completely coupled in the sense that each ATP molecule reacted, leads to transfer of two calcium ions into the reticulum. An alternative process, indicated by step 7 in the diagram, occurs after the

second step when inorganic phosphate leaves the protein, while the energy is dissipated as heat. Calcium ion can leave the reticulum when we add a leak pathway to the membrane. This path is parallel to the transport through the protein and is not indicated in the diagram of Fig.5. Both return pathways results in an *uncoupled* overall process.

The description that follows from this diagram is not satisfactory for one reason in particular. It describes the processes by pure reaction kinetics. Temperature differences and heat flows are not described. As shown by de Meis and others (1997, 2001) the temperature plays an important role (like for instance in thermogenesis), and this description is therefore not thermodynamically satisfactory.

Classical non-equilibrium thermodynamics (de Groot and Mazur 1984, Kjelstrup and others 2006, Kjelstrup and Bedeaux 2008) gives linear relations between the Gibbs energy differences involved and the temperature difference with the reaction rate of ATP, calcium ion flux and heat flux. The linear nature of this description is not satisfactory.

A new methodology has been developed in recent years, with the name of mesoscopic non-equilibrium thermodynamics, to address this problem. Kjelstrup, Rubi and Bedeaux gave in 2005 a first description of the calcium pump, which is nonlinear and contains the temperature as a variable. A short overview of the results is given here, indicating further work in progress.

In equilibrium the reaction Gibbs energy for the ATP conversion,  $\Delta G^i$ , is zero and the chemical potential and temperature outside the membrane,  $\mu_{Ca}^i$  and  $T^i$ , are equal to those in the reticulum,  $\mu_{Ca}^o$  and  $T^o$ . Away from equilibrium this is not the case, and as a result, a reaction rate, calcium ion flux and a total heat flux develop. Both fluxes are positive when they are into the reticulum. Using mesoscopic non-equilibrium thermodynamics we were able to show that

$$r = -D_{rr} \left[ 1 - \exp\left(\frac{\Delta G^i}{RT^i}\right) \right] - D_{rd} \left[ \frac{\mu^o}{RT^o} - \frac{\mu^i}{RT^i} \right] - D_{rq} \left[ 1 - \frac{T^i}{T^o} \right]$$

$$J_{Ca}^o = -D_{dr} \left[ 1 - \exp\left(\frac{\Delta G^i}{RT^i}\right) \right] - D_{dd} \left[ \frac{\mu^o}{RT^o} - \frac{\mu^i}{RT^i} \right] - D_{dq} \left[ 1 - \frac{T^i}{T^o} \right]$$

$$J_q = -D_{qr} \left[ 1 - \exp\left(\frac{\Delta G^i}{RT^i}\right) \right] - D_{qd} \left[ \frac{\mu^o}{RT^o} - \frac{\mu^i}{RT^i} \right] - D_{qq} \left[ 1 - \frac{T^i}{T^o} \right]$$

## Research Projects

In the paper expressions were given for the elements of the  $D$  conductivity matrix in terms of the parameters used in the mesoscopic context. For now it is only needed to know that the matrix is not symmetric.

The important tasks that were solved last year, were to:

- Rewrite the equations using the measurable heat flux  $J_q'$  rather than the total heat flux  $J_q$  and obtain the  $D'$  conductivity matrix using available experimental results. Convert the conductivities into those in the  $D$  matrix using the necessary enthalpies.
- Obtain some of these enthalpies from a first law analysis of the experiments.

Two articles and one chapter (Kjelstrup et al 2008a, 2008b and 2009) were accepted for publication. The aim of these investigations is to eventually describe phenomena like thermogenesis and to learn much about this important and highly efficient element of biological systems. Such knowledge may be useful to develop other efficient chemical processes at the nano level.

*Dick Bedeaux and Signe Kjelstrup*

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## Woman in science and wife of a scientist: Ida Tacke Noddack (1896-1978)

– A research project in the history of chemistry



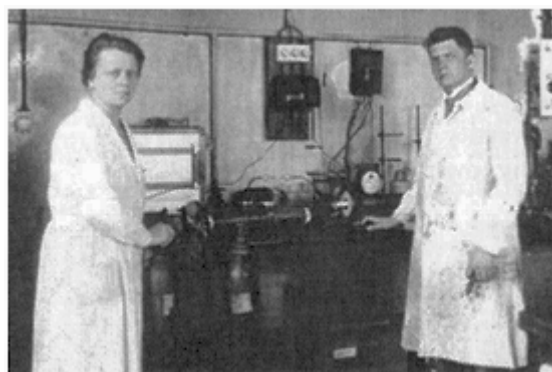
*A woman in science: Ida Tacke Noddack (1896-1978)*

Ida Tacke Noddack (1896-1978) studied chemistry at the Technische Hochschule in Berlin between 1915 and 1921, and was employed as a chemist at Allgemein Elektrizität Gessellschaft (AEG). She resigned to work for free at Siemens-Halske and at the Physikalisch-Technischen Reichsanstalt in Berlin, searching for missing elements 43 and 75. The head of the chemistry department at the Reichsanstalt, Walter Noddack, came to be not only her collaborator, but also her husband from 1926 on.

As a married woman, Tacke Noddack was not longer entitled to a career of her own. In Germany, as in many other countries suffering economically after the First World War women were to leave their positions for the men. Married women, it was argued, were already supported by their husbands and they were needed as housewives whether they had children or not.

However, Ida Noddack was able to continue doing unpaid scientific work, following her husband wherever he was appointed. Through her career Ida

Noddack published about 70 papers, most of them in German and many in collaboration with Walter Noddack. Their most famous joint work dealt with the discovery of elements 43 and 75 and their chemical properties. Eventually the couple was acknowledged for the discovery of element 75 (which they named rhenium after the river Rhine), but their work on element 43 was never recognized.



*The Noddacks: A creative couple*

## Research Projects

Ida Noddack is also known for proposing nuclear fission already in 1934, although she never pursued this topic further. This proposal was never taken seriously in the scientific community. The Noddacks joint work on element 75 however led to three joint Nobel nominations, and another two for Walter Noddack. Ida Noddack was the third woman to be nominated for a Nobel prize, in the good company of Marie Curie and Lise Meitner.

Ida Noddack's career is interesting from many perspectives. She was among the first generation of female students in Germany and among the 1.5% of women that worked in German chemical industry around 1920. As a married woman she had to withdraw from her career, but at the same time, being the wife of a scientist, she enjoyed the privilege of having access to her husband's research facilities and being part of a group of fellow scientists.

Ida and Walter Noddack add to the many "creative couples" in science,<sup>1</sup> such as Marie and Pierre Curie and many less famous couples. Some couples cooperated on all levels of research and shared the honour equally, whereas others were involved in highly asymmetric collaboration. In this study we look at the professional relationship between Ida Noddack and her husband: Were Ida and Walter Noddack equal collaborators? How did they divide the work between them? Is it possible to identify separate research interests and specialities? How did Ida's (and Walter's) work progress as the couple moved from one place (and position) to another?

This research project was initiated in the fall 2007 with Dr. Brigitte Van Tiggelen, research associate of the Université catholique de Louvain, Belgium. The extensive archives of the Noddack couple are held at the Katholieke Universiteit Leuven, Belgium and contain, among other things, correspondence, laboratory notebooks and personal notes. Along with these, we are investigating archives of the places Ida Noddack studied and worked, all of which are located in Germany.



*Annette Lykknes and Brigitte Van Tiggelen investigating manuscripts from the Noddack archives in Leuven.*

Thanks to a substantial grant from the Chemical Heritage Foundation (CHF) in spring 2008 we stayed for one month at the CHF, Philadelphia, USA, to work on this project. At CHF we benefited from an extensive collection of periodicals and books and enjoyed the opportunity to participate in seminars on the history of chemistry on a regular basis. The sojourn allowed us to extend our network and discuss our research with prominent scholars in the field. In September Brigitte Van Tiggelen came to Trondheim to work and lecture at the department, in November our project was presented at the History of Science Society Annual Meeting in Pittsburgh, USA.

The project has received funding from "Anders Jahres fond til vitenskapens fremme".

*Annette Lykknes*

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<sup>1</sup> Helena M. Pycior, Nancy G. Slack and Pnina G. Abir-Am (eds.), *Creative Couples in the Sciences* (New Brunswick, N. J: Rutgers University Press, 1996).

## Writing science – part of an interdisciplinary project on writing competences in all school subjects

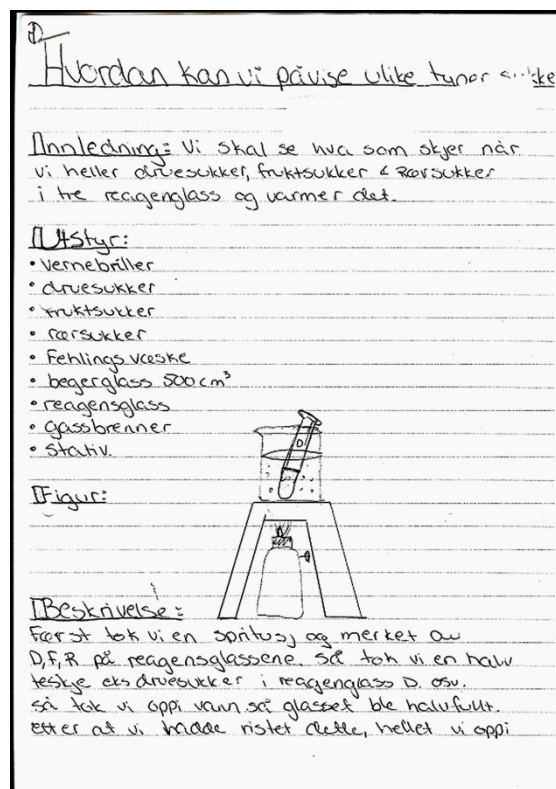
The new curriculum, Kunnskapsløftet, launched in 2006 (hereafter: LK06), introduced five basic skills or competences to be developed in all school subjects. These are: to be able to read, to express oneself in writing, to express oneself orally, to be able to do mathematics and to use digital tools. For a long time the development of writing skills has been a central responsibility for Standard Language Education (mother tongue education). At the same time, writing has been used for several purposes in other school subjects. Traditionally, however, little emphasis has been placed on the texts, genres and the development of writing competences in other school subjects than standard language education. In Norway, this situation changed with LK06, which, as pointed out above, laid more emphasis on writing across the curriculum.

In 2006 a research project on writing as a basic skill in all school subjects from kindergarten to upper secondary school (hereafter SKRIV) was initiated at Sør-Trøndelag University College (HiST), in collaboration with NTNU and Queen Maud's College (DMMH). In 2007 the project was awarded three years of funding from the Norwegian Research Council (NFR). In SKRIV, 22 researchers analyse the conception of writing in "Norwegian", social science/history, religion, mathematics, and science. Special attention is given to the uses and purposes of writing in different subjects at various age levels, drawing on a socio-cultural and social semiotic view of writing.

What does it mean to be able to "express oneself in writing" in science? According to LK06 it includes to present and describe personal experiences of nature, to write experimental reports as well as accounts from excursions and the like, to formulate questions and hypotheses, to employ scientific concepts and expressions, and finally, to present arguments for one's statements. The experimental report is a well-known genre in secondary school science, but what about other genres? How can writing as a basic competence be developed in science, and in what way might writing activities enhance learning in science?

The aim of SKRIV is twofold: to investigate and analyse current practice and prepare teachers for developing writing skills in all school subjects. To help understand and develop writing as a cross-curricular activity, researchers make up interdisciplinary teams. Science is represented by one researcher from faculty for teacher education at HiST and one from the chemistry education group at

Department of Chemistry, NTNU. The study takes a qualitative approach: Each team follows writing activities at different age levels over two years, documenting contexts of writing (including assignments and textbooks) and gathering students' written texts.



Example of students' written texts from our material

This year, our part of the project has been presented at the conferences "FoU i praksis" and "Nordisk konferanse om skrijving som grunnleggende ferdighet og utfordring i utdanning og yrkesliv" in Trondheim, as well as at the 10th Nordic Teacher Trainer Conference in Reykjavik, Iceland. In February the book "Å skrive i alle fag", mainly authored by SKRIV collaborators, was published by Universitetsforlaget. It is aimed at teachers as well as students in teacher education and contains three chapters on writing in science at secondary school level.

Annette Lykknes



# Energikilder

## Ikke-fornybare energikilder

Blant ikke-fornybare energikilder finner vi 2 forskjellige energikilder.

Jeg skal ta for meg de ulike typene. De ikke-fornybare energikildene brukes opp etter hvert.

### Kjernespalting

Ved hjelp av kjernespalting forvandler atomkraftverkene uranbrensel til høyradioaktivt atomavfall. Er lagret inni et hvert atom. I fysikk sies loven det at energi ikke kan oppstå eller forsvinne, men kan forandre form.

Fordelene med Kjernespalting er at det lages store energimengder ut av lite materie. Anleggene tar forholdsvis lite plass om man sammenligner med dammer osv. Og den siste er at selve reaksjonen ikke forurensar.

Den har også sine ulemper, som at det er skadelig stråling fra avfallet. Farlig radioaktivt avfall i mange tusen år fremover.

Dyr i drift og teknologi. Kan være farlig som sikkerheten ikke vektlegges nokk. Og den siste er at den ikke er fornybar, så når stoffet er brukt til fusjon/fisjon kan det ikke nyttes igjen.

### Uran:

Dette er et naturlig grunnstoff med atomnummer 92. Uran er et uedelt metall.

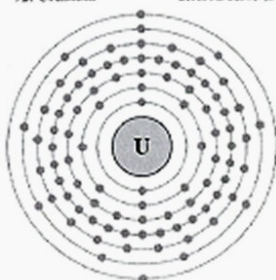
Det var den tyske kjemikeren Martin Heinrich Klaproth som oppdager uran og døpte den etter planeten Uranus.

Uran brukes som brensel i atomreaktorer i kjernekraftverk og ubåter som er atomdrevne. Det brukes også til atomvåpen og til å fremstille radium og plutonium.

Støvet kan sveve i luften i mange timer og ta seg frem mange mil ved hjelp av vinden. Partiklene vir fra seg alfa, beta og gamma. Før bruk blir det knust og malt, før det behandles med syre eller base.

Hvor man skal finne Uran, må man lete både i jordskorpa og i vann. Også i mange bergarter og sedimenter.

92: Uranium 28,18,32,21,9,2



### Fossile energikilder

Fossile energikilder finner man i jordskorpen. Kull, gass og olje er via fotosyntesen omdannet solenergi. Består for det meste av karbon og hydrogen, og av denne grunn svært energifullt.

#### Kull

Dannes stort sett av planterester. Kull har stor økonomisk betydning, og flere land er avhengig av kullkraft for strømproduksjon. Kull inneholder mer oksygen, svovel, nitrogen og mer karbon enn hydrogen i forhold til olje og gass. Kan brukes til direkte oppvarming til prosessindustri og til å lage elektrisitet i et varmekraftverk.

Ulempen med kull er at det blir relativt mye støv sammenlignet med andre fossile brenseltyper.

Derfor blir det betraktet som stor forurensningskilde og årsaker til sur nedbør.

#### Gass

Energiverk som brukes gass som energikilde omdanner høyverdig kjemisk energi i gassen til lavverdig varmeenergi som kan rive turbiner som elektriske generatorer.

Gass inneholder mer hydrogen enn olje, og lite svovel og tungmetaller.

#### Olje

## Chemistry with a Miss

Participation at conferences is a duty for every active chemist as long as NT-faculty grants the money for the expenses. Last June some chemists of the department received some insufficient allocations but with the increment of some legate funds a small delegation was able to undertake the long journey to tropical Okinawa for attending the 15th International Carotenoid Symposium, Fig. 1.



*Fig. 1 Beach of Okinawa*

The participants of such conferences generally share the same interest, they more or less know each other, they attend lectures, scrutinize the posters, conduct the usual small talks: nobody is expecting exciting events. Some suspense may arise when it comes to prize distribution for the best poster.



*Fig. 2 Miss Okinawa*

This happened also in Okinawa. And we were, of course, very happy to hear the conference chairman attributing the prize to PhD-fellow Christer Øpstad. However, such incident would hardly be noteworthy unless the prize is spectacular. Indeed, the prize, a crystal, was brilliant, albeit not breathtaking. Worth





Fig. 3 Award to Vassilia Partali

mentioning are the exceptional circumstances of the price distribution. The award was presented by graceful Miss Okinawa, Figs. 3, 4.



Fig. 4 The distinguished and the distinguisher

Since our delegation comprised two PhD-fellows the other one got increasingly terrified during the awarding ceremony. Would she be distinguished

likewise for her lecture? Fortunately, there were no honors for lectures. Gina Sandru would not have survived a great big hug after a possible prize rewarding by Mister Okinawa, Fig. 5.



Fig. 5 "Mister Okinawa"

Vassilia Partali

## Design of carbon-supported metal-cluster catalysts by molecular dynamics simulations and reactive force fields

Molecular modelling in terms of quantum chemical calculations and molecular dynamics simulations have become an indispensable tool in the design of novel functional materials. In this project, we have used molecular dynamics simulations in conjunction with the reactive force field Reax to study the interactions between graphite and metal clusters. Carbon-supported metal clusters have demonstrated a large catalytic activity and is an alternative to metal surfaces in for example hydrogen production. Clearly, the strong interaction between the carbon surface and the metal clusters (see figure 1) distorts the geometry of the metal cluster leading to an increased catalytic activity. Information is, however, lacking when it comes to an understanding of the mechanisms at an atomistic resolution.

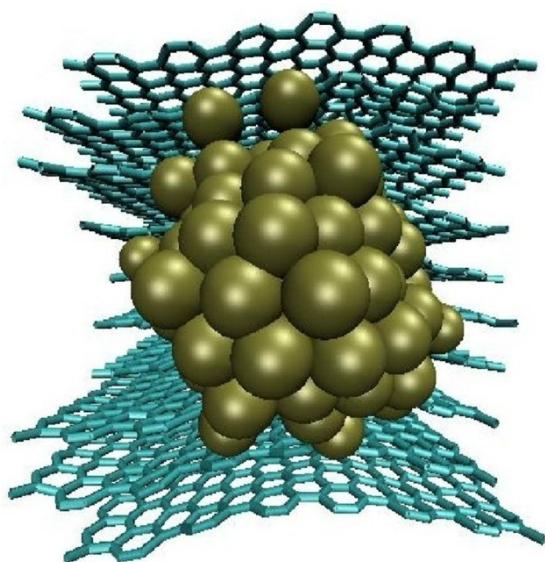


Figure 1.  $Pt_{100}$  cluster interacting with the armchair edge of graphene sheets

In this respect, molecular modeling is a useful tool. In quantum chemistry, the Schrödinger equation is solved for the molecular Hamiltonian providing information about molecular geometries, electric and optical molecular properties, etc. In molecular dynamics simulations, on the other hand, ensemble averages are obtained by calculating the forces between thousands of atoms repeatedly. Typically, the integration time-step is around 1 fs and the simulation is carried out for nanoseconds. Consequently, quantum chemical calculations are normally too expensive for evaluating the forces, and we are limited to force-field methods.

In a force field, the interaction energy is calculated as a sum of various terms: electrostatics, polarization, the van der Waals term (short-range repulsion and dispersion), and intramolecular terms (bond stretching, angle bending and torsional terms). Force fields cannot normally handle chemical reactions, i.e. the breaking and formation

of covalent bonds unless it includes “reactive” features.

In most reactive force fields, a bond-order approach is employed. The bond order for an atom pair is 0 unless the atoms are covalently bonded, it is 1 for a single bond, 2 for a double bond, etc. The bond order for atom  $i$ ,  $BO_i$ , is given as the sum of atom-pair bond orders,  $BO_{ij}$ .

Since atoms in stable molecules are in an oxidation state, only certain values of the atomic bond order are allowed. For carbon, for example, the expected bond order is 4, whereas platinum may have the bond orders 2, 3, 4 and 6. The bond order enters the energy expression in many ways. Over- and under-coordination terms give an energy penalty for deviations from the expected atomic bond orders, i.e., atoms are reactive. Furthermore, the atom-pair bond order is used to turn on (off) intermolecular energy terms at long (short) distances and turn off (on) intramolecular energy terms at long (short) distances.

The most important term in a force field is the electrostatics since it to a large extent governs the properties of the system (polar vs. unpolar molecules, for example). The electrostatics is in most cases represented by atomic charges, and the electrostatic energy is thereby obtained from Coulomb's law. Atomic charges are, however, not transferable from molecule to molecule. For example, the atomic charges in  $F_2$  are zero by symmetry arguments whereas the fluorine charge in HF is highly negative, which demonstrates the difficulties to get transferable atomic charges.

One method to calculate atomic charges on-the-fly in a simulation is the electronegativity equalization method (EEM). The EEM relies on two atom-type parameters, the atomic electronegativity and the atomic chemical hardness. The electronegativity difference between two atoms gives an inherit potential difference which together with the electrostatic potential gives a charge (electron) flow from one atom to another. This charge flow is counter-acted by the chemical hardness (interpreted as the inverse of an atomic capacitance) which gives the work to charge a particle. The EEM gives a linear set of coupled equations to be solved at each step in the simulation to obtain the atomic charges which thus depends on the chemical environment.

We have used the Reax reactive force field as implemented in a parallel (MPI) version of the GRASP molecular dynamics software. We have studied the interactions between metal clusters (Pt and Ni) and carbon surfaces (carbon platelets (see figure 1) and fishbone carbon nanofibers (see figure 2)). For platinum, the force field has been extended by including extra data points from DFT calculations

on small hydrocarbon fragments interacting with a platinum surface. The accuracy of the force field as compared to DFT calculations is demonstrated in figure 3. In general, the deviations are small but significant.

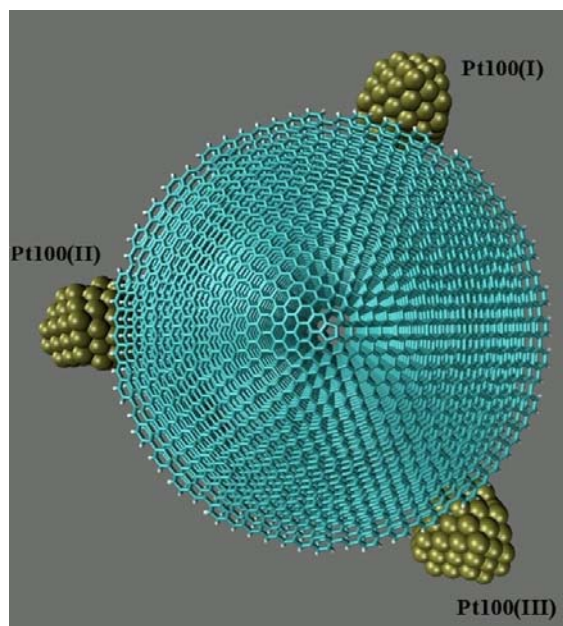


Figure 2. Pt<sub>100</sub> clusters interacting with a fishbone carbon structures.

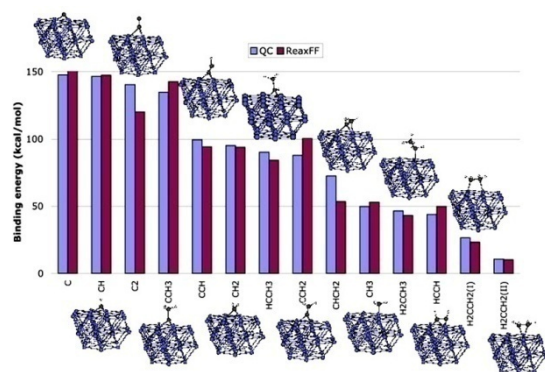


Figure 3. A comparison of the interaction energy as calculated by DFT and by the ReaxFF.

Among the properties we have studied, the Pt-Pt bond length distribution (see figure 4) and the Pt bond-order distribution (see figure 5) are of special interest. For the bond-length distribution, we find that it becomes considerably wider when it interacts with a carbon surface. In particular, the average distance has become longer, which is in agreement with experiments. The bond-order distribution, which has no experimental counterpart, gives more explicit information about the reactivity of the Pt atoms. Normally, the Pt bond-order has some well defined (ideally, integer) numbers, which is the case for the isolated Pt cluster. For the cluster bounded to the carbon surface, the bond-order distribution has lost almost all its structure, indicating that many of the surface atoms are in a reactive state. The same conclusion may be drawn from the bond-length

distribution, based on the strong connection between the bond order and the bond length.

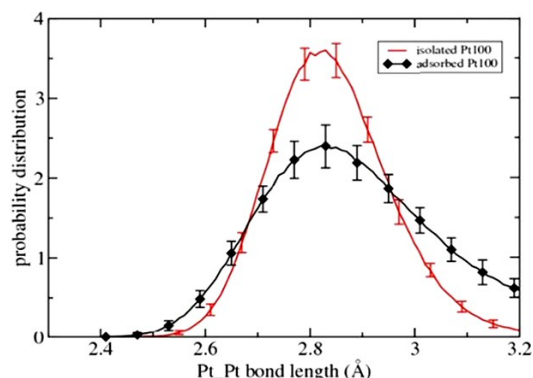


Figure 4. The Pt-Pt bond-length distribution for an unperturbed Pt cluster for a cluster interacting with carbon platelets.

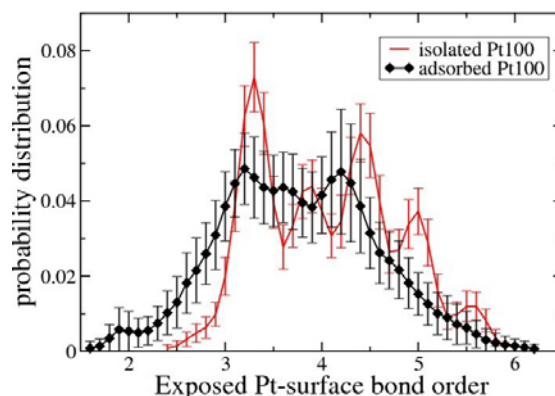


Figure 5. The Pt bond-order distribution for the surface atoms in a cluster.

Per-Olof Åstrand

#### Publications

1. C.F. Sanz-Navarro, P.-O. Åstrand, D. Chen, M. Rønning, A. C. T. van Duin, T. Jacob, W. A. Goddard III, Molecular dynamics simulations of the interactions between platinum clusters and carbon platelets, *J. Phys. Chem. A* 112, 1392-1402, 2008
2. C. F. Sanz-Navarro, P.-O. Åstrand, D. Chen, M. Rønning, A. C. T. van Duin, J. E. Mueller, W. A. Goddard III, Molecular dynamics simulations of carbon-supported Ni clusters using the Reax reactive force field, *J. Phys. Chem. C* 112, 12663-12668, 2008
3. C. F. Sanz-Navarro, P.-O. Åstrand, D. Chen, M. Rønning, A. C. T. van Duin, W. A. Goddard III, Molecular dynamics simulations of metal clusters supported on fishbone carbon nanofibers, submitted for publication



## Honoured with the Order of St. Olav

His Majesty the King has honoured Professor Emeritus Synnøve Liaaen Jensen by appointing her Commander of the The Royal Norwegian Order of St. Olav. This is an order of chivalry that was instituted by King Oscar I of Norway and Sweden on August 21, 1847, as a distinctly Norwegian order. It is named after King Olav II, known for posterity as St. Olav. Commander takes precedence Knight First Class and Knight and is therefore a very special honour for a scientist.



*Photo: Mentz Indergaard/NTNU Info*

The Order was conferred by the County Governor of South-Trøndelag, Kåre Gjønnnes, in a ceremony held in the Council Chamber at NTNU on 30th September 2008..



*Photo: Mentz Indergaard/NTNU Info*

Professor Liaaen Jensen's extensive and internationally recognised research into the chemistry of natural products and the coloured carotenoids



*Photo: Mentz Indergaard/NTNU Info*

In addition, Professor Liaaen Jensen's considerable contribution as a role model for women is recognised by the award.

## Scientific Publications

### Chemistry Dissemination

Eggen, Per-Odd. Eksamen i biologi. Biologididaktikk. Høyskoleforlaget, 2008. ISBN 978-82-7634-595-7. p. 198-214

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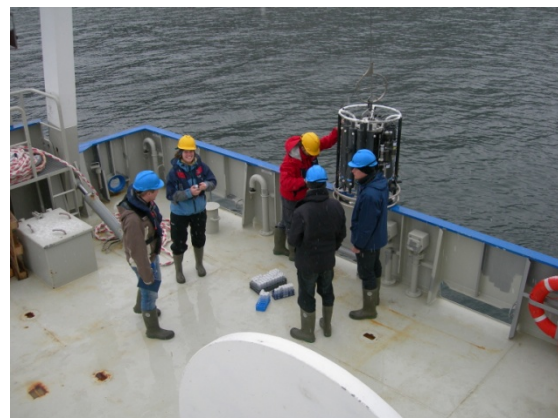
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Galik, Michal; Banica, Ana; Vytras, Karel; Svancara, Ivan; Cesla, Petr; Fischer, Jan; Banica, Florinel Gabriel. Cathodic stripping voltammetry of homocysteine and the respective thiolactone at a mercury electrode. *Chemické listy (Print)* 2008; 102(13): 89

Galik, Michal; Svancara, Ivan; Vytras, Karel; Banica, Florinel Gabriel. Using thiourea as source for electrochemical generation of metal sulfides. *Chemické listy (Print)* 2008; 102(13): 90

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Collecting samples from seawater

Gellein, Kristin; Flaten, Trond Peder; Erikson, Keith M.; Aschner, Michael; Syversen, Tore. Effects of formalin fixation on trace element concentrations in biological tissue. *Cell Biology and Toxicology* 2008; 24(Suppl.1): S101

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## Activities

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Jartun, Morten; Ottesen, Rolf Tore; Steinnes, Eiliv; Volden, Tore. Runoff of particle bound pollutants from urban impervious surfaces studied by analysis of sediments from stormwater traps. *Science of the Total Environment* 2008; 393: 147-163

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*Collecting samples from seawater*

Mariussen, Espen; Steinnes, Eiliv; Breivik, Knut; Nygård, Torgeir; Schlabach, Martin; Kålås, John Atle. Spatial patterns of polybrominated diphenyl ethers (PBDEs) in mosses, herbivores and a carnivore from the Norwegian terrestrial biota. *Science of the Total Environment* 2008; 404(1): 162-170

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## Activities

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*Fishing vessel near Trondheim harbour*

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## Physical Chemistry and Biochemistry

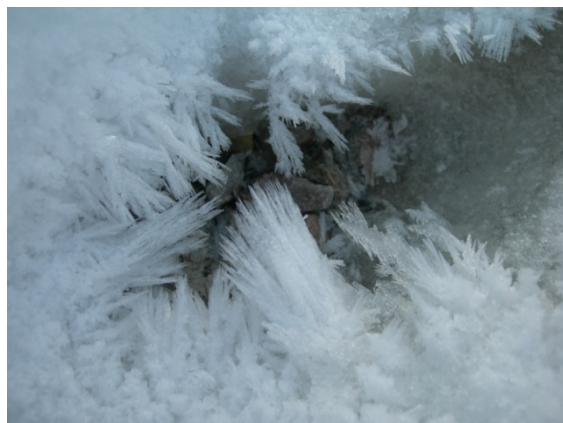
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of bilinear regression models. *Chemometrics and Intelligent Laboratory Systems* 2008; 93(1): 1-10

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## Activities

Lloyd, Seth; Bejan, Adrian; Bennett, Charles; Berretta, Gian Paolo; Butler, Howard; Gordon, Lyndsay; Grmela, Miroslav; Gyftopoulos, Elias P.; Hatsopoulos, George N.; Jou, David; Kjelstrup, Signe; Lior, Noam; Miller, Sam; Rubi, Miguel; Schneider, Eric D.; Sekulic, Dusan P.; Zhang, Zhuomin. Discussion on "Frontiers of the second law". In: Meeting the entropy challenge. American Institute of Physics 2008. ISBN 978-0-7354-0557-8. p. 253-261



*Winter solstice*

Mayer, Alexandre; Lambin, Philippe; Åstrand, Per-Olof. An electrostatic interaction model for frequency-dependent polarizability: Methodology and applications to hydrocarbons and fullerenes. *Nanotechnology* 2008; vol. 19

Mayer, Alexandre; Åstrand, Per-Olof. A Charge-Dipole Model for the Static Polarizability of Nanostructures Including Aliphatic, Olefinic, and Aromatic Systems. *Journal of Physical Chemistry A* 2008; 112: 1277-1285

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boundaries for multiple gels in two-dimensional gel electrophoresis. *Electrophoresis* 2008; 29: 1359-1368

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Sanz-Navarro, Carlos; Åstrand, Per-Olof; Chen, De; Rønning, Magnus; van Duin, Adri C. T.; Jacob, Timo; Goddard III, William A. Molecular Dynamics Simulations of the Interactions between Platinum Clusters and Carbon Platelets. *Journal of Physical Chemistry A* 2008; 112: 1392-1402

Trætteberg, Marit; Kozhushkov, SI; Yufit, DS; de Meijere, A. The structure of tricyclo[3.3.2.0(2.8)]decane (hexahydrobullvalene) - A gas-phase electron diffraction (GED) study. *Journal of Molecular Structure* 2008; 885: 18-22

Zvolinschi, Anita; Kjelstrup, Signe. An indicator to evaluate the thermodynamic maturity of industrial process units in industrial ecology. *Journal of Industrial Ecology* 2008; 12(2): 159-172

Zvolinschi, Anita; Kjelstrup, Signe. Life cycle inventories of energy systems: Results of current systems in Switzerland and other UCTE countries, 2003. *Journal of Industrial Ecology* 2008: vol. 12

Aarset, Kirsten; Hagen, Kolbjørn. Molecular structure and conformation of phenylacetyl chloride as obtained by gas-phase electron diffraction and theoretical calculations. *Journal of Molecular Structure* 2008; 892: 373-377



## Honours, Extracurricular activities, Participation in courses, conferences, lectures and study visits

### B. Alsberg

TV Participation, Schrödingers Katt: "Nytt kamera kan hjelpe politiet", Feb. 2, 2008.

Det 20. norske kjemometrisymposium, Voss, Norway, March 3 – 5, 2008.

Lecture on: The PryJector: A Hyperspectral Projection System.

Visit at Norsk Elektro Optikk AS (NEO), Oslo, Norway, March 6 – 7, 2008.

Linux System Administration Course at LinPro AS, Oslo, Norway, April 21 – 25, 2008.

### T. Andreassen

Conference "23. Organisk kjemisk vintermøte", Geilo, Norway, Jan. 10 – 13, 2008.

Co-author on Poster Presentation: Asymmetric aza-Diels-Alder Reactions of N-Sulfinyl  $\alpha$ -imino Esters.

### T. Anthonsen

Editorial Board Member Journal of Molecular Catalysis, B: Enzymatic.

Chairman Management Committee COST Action D25. Applied Biocatalysis, Stereoselective and Environmentally Friendly Reactions Catalyzed by Enzymes. 22 member countries, 50 research groups

Management Committee Member European Cooperation in Science and Technology. Cascade Chemoenzymatic Processes – New Synergies Between Chemistry and Biochemistry.

Management Committee Meeting "Cascade Chemoenzymatic Processes – New Synergies Between Chemistry and Biochemistry", Como, Italy, September 17 – 21, 2008.

Conference "23. Organisk kjemisk vintermøte", Geilo, Norway, Jan. 10 – 13, 2008.

Co-author on Poster Presentations: "Allosteric Enhancement of Enantioselectivity" and "Chemo-Enzymatic Synthesis of Enantiomerically Pure Haloalcohols".

2nd International Conference Biocatalysis in Non-Conventional Media, Moscow, Russia, June 12 – 15, 2008.

Co-Author on Lecture on: Chemo-Enzymatic Methods for Synthesis of Enantiopure Biologically Active Compounds.

Co-author on Poster Presentation: Biocatalytic Synthesis of Enantiomerically Pure Halohydrins.

ESAB Board Meeting. "Outlining 2009 and 2010 EU FP 7 calls in biocatalysis". Brussels, December 17, 2008

### F.G. Banica

Norwegian Coordinator for International Co-operation Project "Training and Education of Students in Nanotechnology Focused Bioelectrochemistry and Biophysics"; NTNU and Comenius University, Bratislava, Slovak Republic.

Conference "Modern Electrochemical Methods", Usti nad Labem, Czech Republic, May 21 – 23, 2008.

Co-author on Poster Presentation: Thiourea as a Parent Compound for the Electrochemical Generated Sulphid Ion.

19<sup>th</sup> International Conference on Electroanalysis, Prague, Czech Republic, June 16 - 19, 2008.

Co-author on Poster Presentations: "Cathodic Stripping Voltammetry of Homocysteine and the Respective Thiolactone at a Mercury Electrode" and "Using Thiourea as Source for Electrochemical Generation of Metal Sulfides".

Conference "Electrochemistry of Nucleic Acid and Proteins", Brno, Czech Republic, June 19 – 22, 2008.

Co-author on Poster Presentation: Catalytic Hydrogen Evolution in the Presence of Thio-Amino Acids and Ni or Co Ions-new Results Obtained by Cathodic Stripping Voltammetry at a Mercury Electrode.

Research Co-operation at University of Bratislava, Slovak Republic, Nov. 24 – 26, 2008.

### D. Bedeaux

Leave of Absence Jan. 1 – July 31, 2008

Research Stay at Centre for Advanced Study, Oslo, Norway, Jan. 1 – July 31, 2008.

Workshop "Fuel Cell Day", Oslo, Norway, Feb. 7, 2008.

Co-author on Lecture on: Description of the three Phase Contact Line in Non-equilibrium Thermodynamics.

"The Sound of an Equation", Interview in "Impressions", June 1, 2008.

12<sup>th</sup> International ATPase Conference, Aarhus, Denmark, Aug. 5 – 10, 2008.

Co-author on Poster Presentations: "The Heat and Ion Transport of the Ca<sup>2+</sup>-ATPase" and "Heat Transfer through the Ca<sup>2+</sup>-ATPase/Water Interface".

CCP5 Annual Meeting Surfaces and Interfaces, London, UK, Sep. 8 – 10, 2008.

Co-author on Poster Presentation: Heat Transfer through the Ca<sup>2+</sup>-ATPase/Water Interface.

## Activities

### T. Berg

Field Work, Ny-Ålesund, Spitzbergen, March 28 – April 3, June 16 – 30, Aug. 24 – Sep. 1, Oct. 22 – 26 and Nov. 10 – 14, 2008.

21<sup>st</sup> Task Force meeting on the ICP Vegetation, Oulu, Finland, Feb. 26 – 29, 2008.

Co-author on Lecture on: Use of indigenous Moss Samples in Metal Deposition Surveys around Point Sources: Examples from 15 Norwegian Industries.

Workshop “Kongsfjorden System”, Ny-Ålesund, Spitzbergen, March 28 – 30, 2008.

Co-author on Lecture on: Occurrence and Fate of Springtime Atmospheric Deposition of Mercury at Ny-Ålesund.

2<sup>nd</sup> Norwegian Environmental Toxicology Symposium, NTNU, Trondheim, Norway, April 2 – 4, 2008.

Co-author on Poster Presentations: “Speciation, Deposition and Post-Depositional” and “Mercury Levels and Effects in Marine Pelagic Food Webs from Svalbard”.

“Mercury Science at Zeppelin”, TV Participation, Korean Broadcasting System (The Science Café), April 15, 2008.

Lecture on: Mercury in the Arctic, Norwegian Chemical Society, Trondheim, May 7, 2008.

Interview on Internet: Kongelig Zeppelinbesøk, June 26, 2008.

NorthPOP Workshop, St. Petersburg, Russia, May 27 – 29, 2008.

Co-author on Lecture on: Hg in the Arctic.

5<sup>th</sup> SETAC World Congress, Sydney, Australia, Aug. 3 – 7, 2008.

Co-author on Lecture on: Norwegian Measurements of Atmospheric Mercury Depletion Events at Svalbard, Antarctica and the Mainland of Norway.

Co-author on Poster Presentation: COPOL – Contaminants in Polar Regions: Dynamic Range of Contaminants in Polar Marine Ecosystems.

Guest Lectures on: “Forurensninger i atmosfæren” and “Utslipp av luftforurensninger til atmosfæren”, Tromsø, Norway, Sep. 18, 2008.

Guest Lectures on: “Effekter av luftforurensninger” and “Ozonlag og klimaendringer”, Tromsø, Norway, Sep. 19, 2008.

14<sup>th</sup> International Conference on Heavy Metals in the Environment, Taipei, Taiwan, Nov. 16 – 23, 2008.

Co-author on Lecture on: Three Decades of Atmospheric Deposition in Norway Studied by Moss Analysis.

“Terres Arctiques”, TV Participation, French TV5, Dec. 1, 2008.

Conference Arctic Change, Quebec, Canada, Dec. 9 – 12, 2008.

Co-author on Lecture on: Norwegian Measurements of Atmospheric Mercury Depletion Events at Svalbard, Antarctica and the Mainland of Norway.

### M. Bjørgen

Opponent at 3 Doctoral Defences, University of Torino, Italy, Nov. 27 – Dec. 1, 2008.

Visit at University of Oslo, Norway, June 30 – July 4 and Dec. 2 – 9, 2008.

### T. Bruvoll

Norsk kjemometrisymposium, Voss, Norway, March 3 – 5, 2008.

International Supercomputer Conference 2008, Dresden, Germany, June 16 – 20, 2008.



*The southbound coastal express has just left Trondheim harbour 21 September*

### P. – O. Eggen

Conference SAARMSTE 2008, Maseru, Lesotho, Jan. 14 – 18, 2008.

Co-author on Lecture on: Electrifying Chemistry Education from South to North.

NUFU Project, University of Dilla, Ethiopia, Nov. 29 – Dec. 10, 2008.

### A. Fiksdahl

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

Member of National Committee for 18<sup>th</sup> International Conference on Organic Synthesis (ICOS-18) in Bergen, August 2010.

Board Member of the KOSK II Research Program, The Research Council of Norway.

Board Member of “Faggruppen for Organisk kjemi” (the Group of Organic Chemistry) of the Norwegian Chemical Society.

## Activities

Conference “23. Organisk kjemisk vintermøte”, Geilo, Norway, Jan. 10 – 13, 2008.  
Co-author on Lecture on: Synthesis of new  $\beta$ -carboline Analogues.

19<sup>th</sup> annual Florida Heterocyclic and Synthetic Conference, Florida, USA, March 9 – 12, 2008.  
Co-author on Poster Presentation: Synthesis of Novel  $\beta$ -carboline Analogues and Pyridazines.

23<sup>rd</sup> European Colloquium on Heterocyclic Chemistry, Antwerp, Belgium, Sep. 9 – 13, 2008.  
Co-author on Poster Presentation: Pd<sup>II</sup> Complexes of N-aryl-2-Pyridylamines.



*The stairs in Realfagbygget*

### **T.P. Flaten**

Deputy Head of the Department of Chemistry.

Board Member, The Committee for Geomedicine of the Norwegian Academy of Science and Letters.

Editor, Norsk Epidemiologi (Norwegian Journal of Epidemiology).

Conference “Society of Toxicology”, Seattle, USA, March 17 – 20, 2008.  
Co-author on Poster Presentation: Trace Element Profiles in Single Strands of Human Hair.

16<sup>th</sup> Norwegian Epidemiology Conference, Berge, Norway, Nov. 11 – 12, 2008.

Symposium at The Norwegian Academy of Science and Letters, Oslo, Norway, Nov. 13 – 14, 2008.

### **E. Fuglseth**

Conference “23. Organisk kjemisk vintermøte”, Geilo, Norway, Jan. 10 – 13, 2008.  
Co-author on Poster Presentation: Assymmetric Reduction of 4'-Substituted  $\alpha$ -Fluoroacetophenones.

### **O.R. Gautun**

Conference “23. Organisk kjemisk vintermøte”, Geilo, Norway, Jan. 10 – 13, 2008.  
Co-author on Poster Presentations: “Asymmetric aza-Diels-Alder Reactions of N-Sulfinyl  $\alpha$ -imino Esters” and “Asymmetric Catalytic Aziridination of 1,2-Dihydronephthalenes”.

### **K.F. Gebremariam**

Conference SAARMSTE 2008, Maseru, Lesotho, Jan. 14 – 18, 2008.  
Co-author on Lecture on: Electrifying Chemistry Education from South to North.

NUFU Project, University of Dilla, Ethiopia, Nov. 29 – Dec. 15, 2008.

### **K. Gellein**

Conference “Society of Toxicology”, Seattle, USA, March 17 – 20, 2008.  
Co-author on Poster Presentation: Trace Element Profiles in Single Strands of Human Hair.

“En centimeter er nok”, Interview in Gemini, June 1, 2008.

“Hår e meir enn hovudpryd”, Interview on Radio NRK1, June 18, 2008.

### **K.S. Glavatsky**

Fundamentals and Developments of Fuel Cells Conference 2008 – FDFC2008, Nancy, France, Dec. 10 – 12, 2008.  
Co-author on Lecture on: Dynamic Membrane Boundary Conditions for Transport of Heat and Water.

### **S.V. Gonzalez**

7th World Surfactant Congress (CESIO 2008), Paris, France, June 21 – 25, 2008.

17<sup>th</sup> International Symposium on Surfactants in Solution, Berlin, Germany, Aug. 17 – 22, 2008.

### **O. – E. Haas**

Fundamentals and Developments of Fuel Cells Conference 2008 – FDFC2008, Nancy, France, Dec. 10 – 12, 2008.  
Poster Presentation: A Quasi-elastic Neutron Scattering Investigation of the Hydrogen Surface Self Diffusion on Polymer Electrolyte Membrane Fuel Cell Catalyst Support.

## Activities

### K. Hagen

22nd Austin Symposium on Molecular Structure, Austin, Texas, USA, Feb. 29 – March 4, 2008.  
Co-author on Poster Presentations: “Phenylacetyl chloride – Structure and Conformation” and “Conformational and Vibrational Properties of 1,2-Dibromoethyl-Trichlorosilane”.

### Ø. Hestad

Conference ICDL 2008, Poitiers, France, June 30 – July 4, 2008.  
Co-author on Poster Presentation: Streamer Inception in Cyclohexane above and below Freezing Point.

### B.H. Hoff

Conference “23. Organisk kjemisk vintermøte”, Geilo, Norway, Jan. 10 – 13, 2008.  
Co-author on Poster Presentations: “Assymmetric Reduction of 4'-substituted  $\alpha$ -Fluoroacetophenones”, “Allosteric Enhancement of Enantioselectivity” and “Chemo-enzymatic Synthesis of Enantiomerically pure Haloalcohols”.

2<sup>nd</sup> International Conference “Biocatalysis in Non-Conventional Media”, Moscow, Russia, June 11 – 16, 2008.  
Co-author on Poster Presentations: “Regioselective Enzymatic Hydrolysis of Tetrabenzoylated Hexapyranosides” and “Biocatalytic Synthesis of Enantiomerically Pure Halohydrins”.

### S. Ingebrigtsen

16<sup>th</sup> IEEE International Conference on Dielectric Liquids, Poitiers, France, June 30 - July 4, 2008.  
Co-author on Lecture on: Spectral Analysis of Light emitted from Streamers in chlorinated Alkane & Alkane Liquids.  
Co-author on Poster Presentation: “Point Cathode Streamer Propagation in Cyclohexane: Effect of Electron Scavengers” and “Calculation of Ionization Potentials and Electron Affinities for Molecules Relevant for Streamer Initiation and Propagation”.

### I. Inzoli

9<sup>th</sup> International Workshop on State-of-the-Art in Scientific and Parallel Computing, Trondheim, Norway, May 2008.  
7<sup>th</sup> Annual Meeting on High Performance Computing and Infrastructure in Norway (NOTUR 2008), Tromsø, Norway, June 2 – 5, 2008.

Nanostructured Materials & Membranes Training Course, Patras, Greece, June 18 – 27, 2008.

### S.L. Jensen

15th International Symposium on Carotenoids, Okinawa, Japan, June 22 – 27, 2008.  
Co-author on Lecture on: Blue Carotenoids.

Co-author on Poster Presentation: Mechanism for the Carr-Price Blue Colour Reaction of Retinoids.



*The canteen*

### S. Kjelstrup

Leave of Absence Jan. 1 – July 31, 2008

Research Stay at Centre for Advanced Study, Oslo, Norway, Jan. 1 – July 31, 2008.

Geotechnology Colloquia: SPARKS, TU Delft, Netherlands, Jan. 7 – 8, 2008.  
Guest Lecture on: How Can we Better Describe Coupled Heat and Mass Transfer in Natural Processes?

Seminar at the Centre for Advanced Study, Oslo, Norway, Feb. 6, 2008.  
Guest Lecture on: Non-equilibrium Structures: How Can they be Maintained?

2<sup>nd</sup> International Symposium on Biothermodynamics, Frankfurt, Germany, Feb. 21 – 22, 2008.  
Lecture on: Heat Production in Molecular Pumps. How Can we Describe it?

Seminar “New Frontiers in Theory-based Chemical Research”, Oslo, Norway, May 5, 2008.  
Lecture on: Mesoscopic Non-equilibrium Thermodynamics for Biological Systems.

“The Sound of an Equation”, Interview in “Impressions”, June 1, 2008.

Seminar at TU Delft, Department of Process and Energy, June 4, 2008.  
Lecture on: Local Equilibrium – When Does it Apply?

Meeting at Det Norske Veritas, Oslo, Norway, June 16, 2008.  
Guest Lecture on: Nature-inspired Energy Efficient Design.

12<sup>th</sup> International ATPase Conference, Aarhus, Denmark, Aug. 5 – 10, 2008.  
Co-author on Poster Presentations: “The Heat and Ion Transport of the Ca<sup>2+</sup>-ATPase” and “Heat



## Activities

Transfer through the Ca<sup>2+</sup>-ATPase/Water Interface”.

CCP5 Annual Meeting Surfaces and Interfaces, London, UK, Sep. 8 – 10, 2008.  
Co-author on Poster Presentation: Heat Transfer through the Ca<sup>2+</sup>-ATPase/Water Interface.

Member Meeting, Norwegian Chemical Society, Trondheim, Norway, Sep. 9, 2008.  
Guest Lecture on: Onsager lever!

Professor in part time position at TU Delft, Netherlands, Oct. 3 – 17, 2008.

Fundamentals and Developments of Fuel Cells Conference 2008 – FDFC2008, Nancy, France, Dec. 10 – 12, 2008.

Co-author on Lecture on: Dynamic Membrane Boundary Conditions for Transport of Heat and Water.

### H. Koch

Research Stay at Centre for Advanced Study, Oslo, Norway, Jan. 1 – July 31, 2008.

Research Stay at Universidad de Valencia, Spain, Nov. 5 – 11, Nov. 29 – Dec. 11 and Dec. 15 – 22, 2008.

12<sup>th</sup> International ATPase Conference, Aarhus, Denmark, Aug. 5 – 10, 2008.  
Co-author on Poster Presentation: The Heat and Ion Transport of the Ca<sup>2+</sup>-ATPase.



*The entrance hall*

### T. Kumelj

7<sup>th</sup> Annual Meeting on High Performance Computing and Infrastructure in Norway (NOTUR 2008), Tromsø, Norway, June 2 – 5, 2008.

### L. Kvittingen

Conference SAARMSTE 2008, Maseru, Lesotho, Jan. 14 – 18, 2008.

Co-author on Lecture on: Electrifying Chemistry Education from South to North.

Researcher's Night, NTNU, Trondheim, Sep. 26, 2008.

Co-author on Lecture on: e-.

NUFU Project, University of Dilla, Ethiopia, Nov. 29 – Dec. 15, 2008.

### A. Lervik

12<sup>th</sup> International ATPase Conference, Aarhus, Denmark, Aug. 5 – 10, 2008.

Co-author on Poster Presentation: Heat Transfer through the Ca<sup>2+</sup>-ATPase/Water Interface.

CCP5 Annual Meeting Surfaces and Interfaces, London, UK, Sep. 8 – 10, 2008.

Co-author on Poster Presentation: Heat Transfer through the Ca<sup>2+</sup>-ATPase/Water Interface.

### S. Lierhagen

Conference arranged by The Research Council of Norway “Havet og kysten”, Trondheim, Norway, Jan. 29 – 30, 2008.

Co-author on Lecture on: The Chemical Elements in Sediments and Zoobenthos of the Trondheimsfjord in Relation to Wastewater Load.

14<sup>th</sup> International Conference on Heavy Metals in the Environment, Taipei, Taiwan, Nov. 16 – 23, 2008.

Co-author on Lecture on: Influence of Atmospheric Deposition on the Concentration of some Trace Elements in Natural Surface Soil.

### T. Ljones

Conference “23. Organisk kjemisk vintermøte”, Geilo, Norway, Jan. 10 – 13, 2008.

Co-author on Poster Presentation: Allosteric Enhancement of Enantioselectivity.

### A. Lykknes

Research Stay at Chemical Heritage Foundation, Philadelphia, USA, Jan. 18 – Feb. 16, 2008.

Brown Bag Lecture Series, Philadelphia, USA, Jan. 29, 2008.

Co-author on Lecture on: Ida Noddack-Tacke: Woman in Chemistry.

Ukens yrke – kjemiker, [www.utdanning.no](http://www.utdanning.no), Feb. 4, 2008.



## Activities

Participating in Main Excursion for BSc Chemistry and Biochemistry Students at NTNU, Nice, Marseilles and Monaco, France, March 6 – 12, 2008.

Conference "FoU i praksis 2008", Trondheim, April 17 – 18, 2008.

Co-author on Lecture on: Skrivning i naturfag på ungdomstrinnet: Innhold, form og formål.

Conference "10. Nordiske læreruddannelseskongress", Reykjavik, Iceland, May 21 – 24, 2008.

Co-author on Lecture on: Skrivning i naturfag på ungdomstrinnet: Innhold, form og formål.

Ellen Gleditsch: Professor, radiokjemiker og mentor, [www.muv.uio.no](http://www.muv.uio.no), June 2, 2008.

SKRIV Seminar, HiST, Trondheim, Norway, June 2, 2008. Co-author on: Writing Science at Secondary School Level: Content, Form and Purpose.

Conference "6<sup>th</sup> Meeting of STEP", Istanbul, Turkey, June 18 – 22, 2008.

Co-author on Lecture on: Trondheim or Kristiania? An early 20<sup>th</sup> Century Debate on the Education of Industrial Chemists in Norway.

Researcher's Night, NTNU, Trondheim, Sep. 26, 2008.

Co-author on Lecture on: e-.

History of Science Society Annual Meeting, Pittsburgh, PA, USA, Nov. 6 – 9, 2008.

Co-author on Lecture on: Woman of Science and Wife of a Scientist: Ida Noddack-Tacke. (1896-1978).

Nordisk konferanse om skrivning som grunnleggende ferdighet og utfordring i utdanning og yrkesliv, Trondheim, Nov. 17 – 18, 2008.

Co-author on Lecture on: Skrivning i naturfag på 4. og 5. trinn.



*The concave mirror*

### K. Mathisen

Research Stay at the European Synchrotron Radiation Facility (ESRF), Swiss-Norwegian Beam

Line, Grenoble, France, March 12 – 18, July 8 – 17 and Oct. 2 - 9, 2008.

Research Stay at MaxLab, Lund, Sweden, May 14 – 26, 2008.

Workshop "Simultaneous Raman-X-ray Diffraction/Absorption Studies for the in situ Investigation of Solid State Transformations, and Reactions at non ambient Conditions", Grenoble, France, June 18 – 19, 2008.

Poster Presentation: X-ray Absorption and X-ray Powder Diffraction Study on Silver Cluster Formation in Zeolites; Effect of Pore Geometry and Addition of Copper.

Research Stay at Synchrotron Soleil, Paris, France, Oct. 9 - 11, 2008.

### Ø. Mikkelsen

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

Conference about Business Opportunities for the Water Sector for Northern England, Harrogate, UK, Jan. 17, 2008.

Co-author on Lecture on: Unattended Monitoring of Heavy Metals. New Equipment with Methods Making this Possible.

Research stay at the European Synchrotron Radiation Facility (ESRF), Swiss-Norwegian Beam Line (SNBL), Grenoble, France, April 15 – 22 and Nov. 10 – 17, 2008.

IFAT Conference, Munich, Germany, May 5 – 6, 2008.

Conference ESEAC 2008, Prague, Czech Republic, June 15 – 19, 2008.

Co-author on Lecture on: Manganese Detection in River Water by Anodic Stripping Voltametry Using Rotating HG-AG Amalgam Electrode.

Co-author on Poster Presentations: "Continuous Monitoring of Zinc, Iron and Copper in Polluted River Water, Speciation Analyses", "Long Time Monitoring of Zinc and Iron in Waste Water by Use of an Automatic Trace Metal System" and "Nafion Film Coated Silver Amalgam Electrode for Determination of Trace Metals in Presence of Surface Active Compounds".

Meeting "Nasjonalt fagråd ved Universitetet i Oslo", Oslo, Norway, June 18 – 20, 2008.

Researcher's Night, NTNU, Trondheim, Sep. 26, 2008.

Co-author on Lecture on: e-.

University of Seoul, South-Korea, Oct. 7, 2008.

Co-author on Guest Lecture on: Unattended Monitoring of Heavy Metals. New Methods Making this Possible with the SensAqua ATMS500 Equipment.

## Activities

Conference, Exhibition and Workshops on Water, Wastewater & Environmental Monitoring (WWEM), Telford, UK, Nov. 5 – 6, 2008.

Co-author on Lecture on: Remote and Unattended Monitoring of Heavy Metals in Waters. Requirements for such Monitoring and how this Can be Done Automatically.

Committee Member at Doctoral Defence Ludovic Lesven, University of Science and Technology Lille, France, Dec. 1 – 4, 2008.



*From the botanical garden*

### **D.G. Nicholson**

Head of the Department of Chemistry

Meeting and Projects at North West University, South Africa, Feb. 1 – 14, 2008.

Research stay at the European Synchrotron Radiation Facility (ESRF), Swiss-Norwegian Beam Line (SNBL), Grenoble, France, April 9 – 13, June 17 – 20 and July 8 – 15, 2008.

Research Stay at MaxLab, Lund, Sweden, May 19 – 23, 2008.

Committee Meeting NWO (The Research Council of Netherlands), The Hague, Netherlands, May 29 – 30, 2008.

SNX Council Meeting (SNBL), Annecy, France, June 2 – 6, 2008.

Workshop on Raman Spectroscopy and Experiment Planning, SNBL, Grenoble, France, June 17 – 20, 2008.

Organising Seminar (SNBL), La Fauvelle, France, Sep. 8 – 15, 2008.

SNX Council Meeting (SNBL), Grenoble, France, Nov. 25 – 29, 2008.

### **M. Nordløy**

14<sup>th</sup> International Conference on Heavy Metals in the Environment, Taipei, Taiwan, Nov. 16 – 23, 2008.

Co-author on Lecture on: Concentrations of 46 Elements in Natural Vegetation in Norway: Seasonal Trends.

### **V. Partali**

15<sup>th</sup> International Symposium on Carotenoids, Okinawa, Japan, June 22 – 27, 2008.

Co-author on Poster Presentations: “Inherently Colored Soaps”, “Fungal Hydrolysis of Crocin”, “Oxidation and Antioxidation of Carotenoids – Reaction and Products”, “Carotenoid Aggregates of Predefined Size”, “Easy Synthesis of Stable Anionic Carotenoid Radicals” and “Cationic Carotenoid Amphiphiles as Gene Transfection Vectors”.

Co-author on Lecture on: Carotenoid Compounds Out of the Ordinary.

ESF Workshop “Novel Methods in Exploring Carotenoid Excited State Dynamics”, Nove Hradý, Czech Republic, Sep. 21 – 25, 2008.

Co-author on Poster Presentation: Excited-state Properties of Hydrophilic Carotenoids.

### **A.L. Ramstad**

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

Excursion Leader, Main Excursion for BSc Chemistry and Biochemistry Students at NTNU, Nice, France, March 6 – 12, 2008.

Research Stay at the European Synchrotron Radiation Facility (ESRF), Swiss-Norwegian Beam Line, Grenoble, France, April 15 – 22 and Nov. 9 – 14, 2008.

### **E. – M. Sandru**

15<sup>th</sup> International Symposium on Carotenoids, Okinawa, Japan, June 22 – 27, 2008.

Co-author on Lecture on: Carotenoid Compounds out of the Ordinary.

Co-author on Poster Presentation: Carotenoid Aggregates of Predefined Size.

### **K. Schröder**

Conference about Business Opportunities for the Water Sector for Northern England, Harrogate, UK, Jan. 17, 2008.

Co-author on Lecture on: Unattended Monitoring of Heavy Metals. New Equipment with Methods Making this Possible.

University of Seoul, South-Korea, Oct. 7, 2008.

Co-author on Guest Lecture on: Unattended Monitoring of Heavy Metals. New Methods Making this Possible with the SensAqua ATMS500 Equipment.

Conference, Exhibition and Workshops on Water, Wastewater & Environmental Monitoring (WWEM), Telford, UK, Nov. 5 – 6, 2008.

Co-author on Lecture on: Remote and Unattended Monitoring of Heavy Metals in Waters.

## Activities

Requirements for such Monitoring and how this Can be Done Automatically.

### N. Simic

Bruker User Meeting and the 10<sup>th</sup> National NMR Meeting, Oppdal, Norway, Jan 15 – 18, 2008.

Field Work, Niš, Serbia, July 7 – 11, 2008.

### S. Skogvold

Research Stay at the European Synchrotron Radiation Facility (ESRF), Swiss-Norwegian Beam Line, Grenoble, France, April 15 – 22 and Nov. 10 – 17, 2008.

Conference ESEAC 2008, Prague, Czech Republic, June 15 – 19, 2008.

Co-author on Lecture on: Manganese Detection in River Water by Anodic Stripping Voltametry Using Rotating HG-AG Amalgam Electrode.

Researcher's Night, NTNU, Trondheim, Sep. 26, 2008.

Co-author on Lecture on: e-

### H.S. Smalø

16<sup>th</sup> IEEE International Conference on Dielectric Liquids, Poitiers, France, June 30 -July 4, 2008.  
Co-author on Poster Presentation: Calculation of Ionization Potentials and Electron Affinities for Molecules Relevant for Streamer Initiation and Propagation.



View from the cathedral

### A.O. Steen

TV Participation, NRK1 Schrödingers Katt: "Kvikksølvforurensning", Jan. 24, 2008.

"Fjerne miljøsynder avsløres på Svalbard", Interview in Adresseavisen, Feb. 21, 2008.

TV Participation, Euro News: "Scientists Research Falling Mercury", March 13, 2008.

Workshop "Kongsfjorden System", Ny-Ålesund, Spitzbergen, March 28 – 30, 2008.

Co-author on Lecture on: Occurrence and Fate of Springtime Atmospheric Deposition of Mercury at Ny-Ålesund.

2<sup>nd</sup> Norwegian Environmental Toxicology Symposium, NTNU, Trondheim, Norway, April 2 – 4, 2008.

Co-author on Poster Presentation: Speciation, Deposition and Post-Depositional.

Field Work, Ny-Ålesund, Spitzbergen, Feb. 21 – March 7, June 15 – 23 and July 6 – 17, 2008.

TV Participation: "Terres Arctiques", French TV5, Dec. 1, 2008.

### E. Steinnes

6<sup>th</sup> International Symposium on modern Principles of Air Monitoring, Geilo, Norway, Jan. 28 – 31, 2008.  
Lecture on: Atmospheric Deposition of Metals Around some Industrial Plants in Norway Studied by Moss Analysis.

Conference arranged by The Research Council of Norway "Havet og kysten", Trondheim, Norway, Jan. 29 – 30, 2008.

Co-author on Lecture on: The Chemical Elements in Sediments and Zoobenthos of the Trondheimsfjord in Relation to Wastewater Load.

21<sup>st</sup> Task Force meeting on the ICP Vegetation, Oulu, Finland, Feb. 26 – 29, 2008.

Co-author on Lectures on: "Use of Indigenous Moss Samples in Metal Deposition Surveys Around Point Sources: Examples from 15 Norwegian Industries" and "Experience from the Use of Reference Samples in the 2005/2006 Moss Survey".

Det 17. nasjonale seminar om hydrogeologi og miljøkjemi, NGU, Trondheim, March 11 – 12, 2008.  
Lecture on: Lead in the Norwegian Environment: Contribution from Natural and Anthropogenic Sources.

2<sup>nd</sup> International Nuclear Chemistry Congress, Cancun, Mexico, April 13 – 18, 2008.

Co-author on Lecture on: Radiocesium Fallout in Norway from the Chernobyl Accident: Impact on Terrestrial Ecosystems and new Knowledge Acquired.

Conference "Radioecology & Environmental Radioactivity", Bergen, Norway, June 15 – 20, 2008.



## Activities

Co-author on Lecture on: Geographical Trends in 137Cs Fallout from the Chernobyl Accident and Leaching from Natural Surface Soil in Norway.

33<sup>rd</sup> International Geological Congress, Oslo, Norway, Aug. 6 – 14, 2008.  
Lecture on: Soils and Geomedicine.

Conference EUROSOIL 2008, Vienna, Austria, Aug. 25 – 29, 2008.  
Lecture on: Soils and Geomedicine.

4<sup>th</sup> National Conference on Applied Physics, Romanian Physics Society, Sep. 25 – 26, 2008.  
Lecture on: 30 years of Air Pollution Studies in Norway Using INAA and ICP-MS.

14<sup>th</sup> International Conference on Heavy Metals in the Environment, Taipei, Taiwan, Nov. 16 – 23, 2008.  
Co-author on Lectures on: “Distribution of 28 Elements in Podzol Profiles Studied by Fractional Extractions and Multivariate Statistics”, “Influence of Atmospheric Deposition on the Concentration of some Trace Elements in Natural Surface Soil”, “Concentrations of 46 Elements in Natural Vegetation in Norway: Seasonal Trends” and “Three Decades of Atmospheric Deposition in Norway Studied by Moss Analysis”.

### V. Stockmann

Conference “23. Organisk kjemisk vintermøte”, Geilo, Norway, Jan. 10 – 13, 2008.  
Co-author on Lecture on: Synthesis of new  $\beta$ -carboline Analogues.

19<sup>th</sup> annual Florida Heterocyclic and Synthetic Conference, Florida, USA, March 9 – 12, 2008.  
Co-author on Poster Presentation: Synthesis of Novel  $\beta$ -carboline Analogues and Pyridazines.

### K. Strasunskiene

Research Stay at University of Science and Technology of Lille, France, Jan. 7 – 31, 2008.

Conference ESEAC 2008, Prague, Czech Republic, June 15 – 19, 2008.  
Co-author on Poster Presentations: “Long Time Monitoring of Zinc and Iron in Waste Water by Use of an Automatic Trace Metal System” and “Nafion Film Coated Silver Amalgam Electrode for Determination of Trace Metals in Presence of Surface Active Compounds”.

### C.L. Øpstad

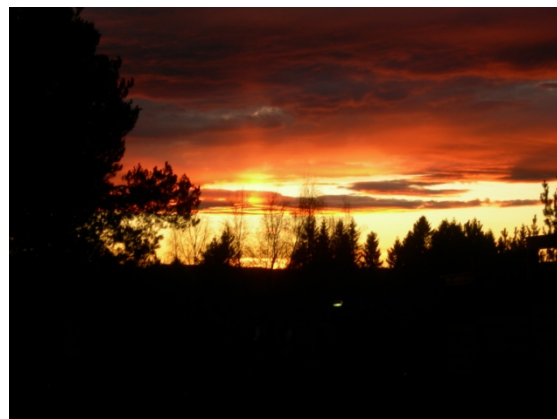
15<sup>th</sup> International Symposium on Carotenoids, Okinawa, Japan, June 22 – 27, 2008.  
Co-author on Lecture on: Carotenoid Compounds out of the Ordinary.  
Co-author on Poster Presentations: “Easy Synthesis of Stable Anionic Carotenoid Radicals” and “Cationic Carotenoid Amphiphiles as Gene Transfection Vectors”.

Research Stay at Weill Cornell Medical College in Quatar, Doha, Quatar, Sep. 27 – Oct. 12, 2008.

### J.E. Aaseng

Conference “23. Organisk kjemisk vintermøte”, Geilo, Norway, Jan. 10 – 13, 2008.  
Co-author on Poster Presentation: Asymmetric Catalytic Aziridination of 1,2-dihydronaphthalenes.

19<sup>th</sup> annual Florida Heterocyclic and Synthetic Conference, Florida, USA, March 9 – 12, 2008.  
Poster Presentation: Substituted (*/S*)-2-Aminotetralins from L-Aspartic Acid.



*Sky on fire*

### P. – O. Åstrand

Research Co-operation at Northwestern University, Illinois, USA, March 1 – 9, 2008.

Guest Lecture on: Molecular Mechanics Models for Linear and Nonlinear Electronic Polarization, at Northwest University, Evanston, Illinois, USA, March 6, 2008.

Research Co-operation at The Pennsylvania State University, USA, March 9 – 19, 2008.

PARA 2008: 9<sup>th</sup> Workshop on State-of-the Art in Scientific and Parallel Computing, NTNU, Trondheim, May 13 – 16, 2008.  
Lecture on: Molecular Modelling: Basic Concepts and Applications in Catalysis.

16<sup>th</sup> IEEE International Conference on Dielectric Liquids, Poitiers, France, June 30 - July 4, 2008.  
Co-author on Poster Presentations: “Point Cathode Streamer Propagation in Cyclohexane: Effect of Electron Scavengers” and “Calculation of Ionization Potentials and Electron Affinities for Molecules Relevant for Streamer Initiation and Propagation”.

1<sup>st</sup> Nanotechnology@NTNU, NTNU Nanolab., Trondheim, Sep. 11 - 12, 2008.  
Co-author on Lecture on: Engineering of Metal Nanoparticles on Carbon Nanofibers.



**Spring examination**

<b>Course no.</b>	<b>Course title (credits)</b>	<b>Lectures and exercise coordinators</b>	<b>Candidates/ Passed</b>
RFEL1001	Natural Science and World Views (7,5)	Reidar Edvald Stølevik Karl Erik Zachariassen	72/65
KJ1020	Organic Chemistry (15)	Vassilia Partali	140/118
KJ2022	Spectroscopic Methods in Organic Chemistry (7,5)	Nebojsa Simic	17/15
KJ2041	Physical Chemistry II (7,5)	Reidar Edvald Stølevik	13/11
KJ2043	Physical Methods in Structural Chemistry (15)	Astrid Lund Ramstad Reidar Edvald Stølevik	6/6
KJ2051	Analytical Chemistry, Advanced Course (7,5)	Øyvind Mikkelsen Florinel Gabriel Banica	5/5
KJ2053	Chromatography (7,5)	Anne Fiksdahl Rudolf Schmid	29/29
KJ2070	Environmental Chemistry (15)	Torunn Berg Trond Peder Flaten	39/32
KJ3055	Analytical Atomic Spectrometry (7,5)	Florinel Gabriel Banica	2/2
KJ3065	Enzyme chemistry (7,5)	Torbjørn Ljones	9/9
KJ8100	Organic Medicinal and Pharamaceutical Chemistry (7,5)	Derek James Chadwick	8/8
KJ8106	Advanced Organic Chemistry (7,5)	Per Henning Carlsen	-
KJ8200	Spectroscopy and Chemometrics (7,5)	Bjørn Kåre Alsberg	-
KJ8204	Quantitative Structure-Activity Relationships (7,5)	Bjørn Kåre Alsberg	2/2
KJ8205	Molecular Modelling (7,5)	Per-Olof Åstrand	3/3
KJ8208	Advanced Irreversible Thermodynamics (6)	Signe Kjelstrup	-
TKJ4111	Organic Chemistry, Advanced Course (7,5)	Bård Helge Hoff	17/17
TKJ4130	Organic Synthesis, Laboratory (7,5)	Odd Reidar Gautun Anne Fiksdahl	8/8
TKJ4135	Organic Synthesis, Advanced Course (7,5)	Odd Reidar Gautun	10/7
TKJ4145	Industrial Organic Chemistry, Research Projects (7,5)	Bård Helge Hoff	10/10
TKJ4160	Basic Physical Chemistry and Laboratory (15)	Morten Bjørgen Per-Olof Åstrand	84/75
TKJ4166	Chemical Bond Theory and Spectroscopy (7,5)	Mats Linus Henrik Boman	19/15
TKJ4175	Chemometrics, Basic Course (7,5)	Bjørn Kåre Alsberg	2/2
TKJ4190	Physical Chemistry, Project Work (7,5)	Terje Bruvoll	5/5
TKJ4850	Experts in Team, Interdisciplinary Project (7,5)	Per-Olof Åstrand	18/18



Autumn view of Trondheim

**Autumn examination**

<b>Course no.</b>	<b>Course title (credits)</b>	<b>Lectures and exercise coordinators</b>	<b>Candidates/ Passed</b>
KJ1000	General Chemistry (15)	Lise Kvittingen Torbjørn Ljones Annette Lykknes	193/153
KJ1030	Inorganic Chemistry (15)	Astrid Lund Ramstad	32/26
KJ1040	Physical Chemistry (15)	Morten Bjørgen Astrid Lund Ramstad Florinel Gabriel Banica	28/19
KJ2031	Inorganic Chemistry, Advanced Course (7,5)	Karina Mathisen	9/9
KJ2050	Analytical Chemistry, Basic Course (7,5)	Øyvind Mikkelsen Florinel Gabriel Banica	25/25
KJ2090	Chemistry Education - Chemistry Dissemination (7,5)	Per Odd Eggen	3/2
KJ2091	Teacher training/dissemination project in chemistry (7,5)	Lise Kvittingen	-
KJ3021	Nuclear Magnetic Resonance Spectroscopy (7,5)	Nebojsa Simic	16/15
KJ3058	Analytical Chemical Separation Techniques (7,5)	Rudolf Schmid	-
KJ3071	Applied geochemistry (7,5)	Rolf Tore Ottesen	15/15
RFEL3093	Episodes from the history of science	Annette Lykknes	10/10
RFEL8093	Episodes from the history of science	Annette Lykknes	-
KJ8021	Stereochemistry and Synthesis of Chiral Compounds (7,5)	Per Henning Carlsen	1/1
KJ8052	Analytical Electrochemistry and its Application within Industrial and Environmental Monitoring (7,5)	Øyvind Mikkelsen	6/6
KJ8056	Chemical and Sensors and Biosensors (7,5)	Florinel Gabriel Banica	5/5
KJ8070	Advanced Aquatic Chemistry (15)	Trond Peder Flaten	9/9
KJ8104	New Methods in Organic Synthesis (7,5)	Anne Fiksdahl	8/8
KJ8105	Organometallic Compounds in Organic Synthesis (7,5)	Odd Reidar Gautun	-
KJ8106	Advanced Organic Chemistry	Per Henning Carlsen	-
KJ8206	Advanced Quantum Chemical Methods (7,5)	Henrik Koch	-
KJ8207	Advanced Microarray Data Analysis (7,5)	Bjørn Kåre Alsberg	9/8
TKJ4100	Basic Organic Chemistry and Laboratory (15)	Per Henning Carlsen	79/60
TKJ4170	Quantum Chemistry, Advanced Course (7,5)	Henrik Koch	7/7
TKJ4180	Physical Organic Chemistry (7,5)	Rudolf Schmid	13/10
TKJ4195	Chemometrics, Advanced Course (7,5)	Bjørn Kåre Alsberg	-
TKJ4200	Irreversible Thermodynamics (7,5)	Signe Kjelstrup	4/4
TKJ4205	Computational Chemistry (7,5)	Per-Olof Åstrand	7/7
TKJ4215	Statistical Thermodynamics in Chemistry and Biology (7,5)	Per-Olof Åstrand	24/24
TKJ4510	Physical Chemistry, Specialization Project (15)	Morten Bjørgen	4/3
TKJ4515	Physical Chemistry, Specialization Course (7,5)	Morten Bjørgen	4/4
TKJ4520	Organic Chemistry, Specialization Project (15)	Odd Reidar Gautun	8/8
TKJ4525	Organic Chemistry, Specialization Course (7,5)	Anne Fiksdahl	16/15

## Re-sit examination

Course no.	Course title (credits)	Candidates/ Passed
RFEL1001	Natural Science and World Views (7,5)	33/29
KJ1000	General Chemistry (15)	8/6
KJ1020	Organic Chemistry (15)	11/5
KJ1030	Inorganic Chemistry (15)	3/1
KJ1040	Physical Chemistry (15)	1/1
KJ2022	Spectroscopic Methods in Organic Chemistry (7,5)	3/3
KJ2043	Physical Methods in Structural Chemistry (15)	1/1
KJ2050	Analytical Chemistry, Basic Course (7,5)	2/2
KJ2070	Environmental Chemistry (15)	3/2
KJ2090	Chemistry Education - Chemistry Dissemination (7,5)	1/1
KJ3021	Nuclear Magnetic Resonance Spectroscopy (7,5)	2/1
KJ8026	Biocatalysis in Organic Chemistry (7,5)	2/2
KJ8056	Chemical and Sensors and Biosensors (7,5)	1/1
KJ8206	Advanced Quantum Chemical Methods (7,5)	1/1
TKJ4100	Basic Organic Chemistry and Laboratory (15)	18/3
TKJ4135	Organic Synthesis, Advanced Course (7,5)	1/1
TKJ4160	Basic Physical Chemistry and Laboratory (15)	4/1
TKJ4166	Chemical Bond Theory and Spectroscopy (7,5)	1/0



*Wild pansy (Viola tricolor) in May*

### Siv.ing. students

#### 3. year (MTKJ)

Austdal, Marie  
Blakstad, Guro  
Bugge, Steffen  
Bøe, Maren Seljenes  
Gulbrandsen, Tore Aarhus  
Kaasa, Kristin  
Nerem, Elisabeth  
Solvang, Tina  
Tungen, Jørn Eivind  
Tveiekrem, Marit Elise Endresen

#### 4. year (MTKJ)

Lyngvi, Eirik  
Mekki, Miriam  
Rognså, Guro Helgesdotter  
Seglem, Karen Nessler  
Slungård, Sigrid Volden  
Takla, Marit  
Vågenes, Birgitte Bårli  
Willassen, Veronica

#### 5. year (MTKJ)

Berg, Michel Brunes  
Krakeli, Tor Arne  
Kvalvåg, Sondre Schnell  
Landsem, Eva  
Mui, Vivian Wing Laam  
Poon, Cheau Ling  
Ringholm, Magnus  
Strand, Lilian Helene Sola  
Sørensen, Benedicte Riise  
Sørum, Christopher  
Voldsund, Mari  
Wilhelmsen, Øivind  
Åstrand, Ove Alexander

### Master students in progress

#### Chemistry (MKJ)

Berge, May Britt  
Berge, Øystein Rønning  
Bøyese, Katrine Lie  
Delic, Asmira  
Edwardsen, Tove-Nanny  
Egede-Nissen, Cecilie  
Grave, Anlaug Haukvik  
Haug, Siri  
Helgerud, Trygve  
Hoftaniska, Idar  
Holt, Yngvil  
Hovde, Gunnhild  
Hystad, Madeleine  
Jonassen, Hilding  
Kaspersen, Svein Jacob  
Kristiansen, Tina  
Lie, Aleksander  
Næss, Mari Kirkebøen  
Siegesmund, Øyvind Torbjørn  
Sivertsen, Sveinung Sundfør  
Skorpa, Ragnhild  
Sveinhaus, Krister  
Thvedt, Thor Håkon Krane  
Tynes, Mari Klevberg  
Valvik, Beate  
Volynkin, Andrey Sergeevich  
Aaen, Ingrid

#### Environmental toxicology and chemistry (MFORU)

Ottemo, Vivian Grønhaug

#### Master of Science Education (MLREAL)

Dahl, Anette  
Sæth, Erlend Solveigson



At the laboratory, Photo: Svein Erik Dahl



**The following PhD-projects are in progress:**

<b>Student</b>	<b>Title</b>	<b>Thesis advisor</b>
Angelsen, Ragnhild B. Strand	Heterocyclic synthetic chemistry based on nitropyridine derivatives.	Anne Fiksdahl
Burheim, Odne Stokke	Elektronisk utfelling av jern. (Electrowinning of iron from chloride melts.)	Signe Kjelstrup
Chu, Chunmei	Automated <i>de novo</i> optimization of functional organometallic compounds by integrating a QSAR/genetic algorithm method.	Bjørn K. Alsberg
Eggen, Per-Odd	Current chemistry – learning and teaching electrochemistry by experiments.	Lise Kvittingen
Esmurziev, Aslan	Synthesis of new fluorinated uronic acids and total synthesis of new uridine diphosphate fluoro-uronic acids. (Syntese av fluorerte uronsyrer og talsyntes av nye uridine difosfat fluoro-uronsyrer.)	Bård Helge Hoff
Flatberg, Arnar	Simulation of microarray experiments and protsomic 2D gel electrophoresis.	Bjørn K. Alsberg
Fuglseth, Erik	New chiral and fluorinated aromatic compounds. (Nye kirale og fluorere aromatiske forbindelser.)	Bård Helge Hoff
Gebremariam, Kidane Fanta	Analytical methods for art objects investigation	Lise Kvittingen
Glavatsky, Kirill Sergeevich	Multi-component evaporation as described using the nonequilibrium van der Waals square gradient model.	Dick Bedeaux
Gonzalez, Susana Villa	Synthesis of optically active surfactants and the study of their properties.	Per H. Carlsen
Haas, Ole-Erich	Transport on a nanoscale; at surfaces and contact lines in PEM fuel cells.	Astrid Lund Ramstad
Ham, Leen van der	Optimising the Second law efficiency of a cryogenic air separation unit	Signe Kjelstrup
Hestad, Øystein Leif	Elektroniske prosesser i frosne dielektriske væsker under høy elektrisk felt påkjenning.	Per-Olof Åstrand
Iftekhhar, Shafia	Trace metals and natural organic matters in rivers.	Torunn Berg
Kumelj, Tjasa	Free energy calculations of ligand-protein interactions.	Per-Olof Åstrand
Lervik, Anders	Energy transfer in biomolecular motors	Signe Kjelstrup
Løkken, Torbjørn Vegard	Analyser av vannduggpunkt og hydrokarbonduggpunkt i naturgass. (Determination of water dewpoint and hydrocarbon dew-point in natural gas.)	Rudolf Schmid
Melnes, Silje	Rational drug design synthesis of potential selective inhibitors of tyrosin kinase 2.	Odd Reidar Gautun

## Post Graduate Students

Mohsin, Muhammad Ali	Surface functionalization by bio-organic materials.	Florinel G. Banica
Nordløyken, Marit	Spormetaller i hjortedyr i Norge. (Trace of elements in Norwegian deer).	Torunn Berg
Ryeng, Einar	Analyse av mikromatrisedata med induktiv logikk-programmering.	Bjørn K. Alsberg
Sandru, Eugenia-Mariana	Syntese av høy umettete bioorganiske forbindelser. (Synthesis of highly unsaturated bioorganic compounds.)	Vassilia Partali
Smalø, Hans Sverre	Molecular models of electronic processes in liquids.	Per-Olof Åstrand
Steen, Anne Orderdalen	Atmosfærisk spesiering av kvikksølv i polare områder.	Torunn Berg
Stockmann, Vegar	Synthetic applications of nitropyridine derivatives.	Anne Fiksdahl
Strasunskiene, Kristina	Automatically measuring systems for heavy metals and trace metals in waste water from sewage discharge and incineration plants. Early warning systems.	Øyvind Mikkelsen
Syed, Majid Bukhari	Isolation and structure elucidation of natural Bioactive molecules of plant origin.	Nebojsa Simic
Xu, Jing	A nonequilibrium molecular dynamics simulation study of chemical reactors.	Signe Kjelstrup
Zaidi, Asma	Synthesis of highly unsaturated amino acids.	Vassilia Partali
Zeeshan, Muhammad	Optical resolution by fractional aggregation.	Vassilia Partali
Øpstad, Christer Lorentz	Synthesis and properties of hydrophilic highly unsaturated amphiphiles for gene transfer.	Vassilia Partali
Aarhaug, Thor Anders	Ny membran for polymer brenselceller.	Signe Kjelstrup
Aaseng, Jon Erik	Asymmetric synthesis of substituted 2-aminotetralins. (Asymmetrisk syntese av substituerte 2-aminotetraliner.)	Odd Reidar Gautun



Gråkallen – late autumn

## MSc in Chemistry 2008

Alsvik, Inger Lise Supervisor: Examiners:	Inherently colored soaps. Professor Vassilia Partali Associate Professor Birte Sjursnes, HiØ Associate Professor Eva Mørkved
Eliassen, Ragnhild Oline Supervisors: Examiners:	Epifyttisk lav som indikator på luftforurensning i Sør-Varanger. Professor Eiliv Steinnes Research Manager Inga Bruteig, NINA Professor Else Løbersli, DN Professor Øyvind Mikkelsen
Helland, Tone Grangård Supervisors: Examiners:	Selected pharmaceutical residues in Norwegian sewage effluent and the adjacent aqueous environment. Professor Torunn Berg Associate Professor Roland Kallenborn, UNIS Senior Research Scientist Per Johan Brandvik, SINTEF Associate Professor Rudolf Schmid
Hermann, Solveig Supervisors: Examiners:	Utvikling av automatisk målesystem for sink, kadmium og kvikksølv i avløpsvann fra forbrenningsanlegg. Professor Øyvind Mikkelsen Stipendiat Silje Marie Skogvold Stipendiat Kristina Strasunskiene Professor Emeritus Knut Schrøder
Kjøglum, Kristin Tyldum Supervisors: Examiners:	Sensor development for environmental and industrial process monitoring. Development of solid state electrodes for surveillance of scale components in produced water from oil production. Professor Øyvind Mikkelsen Stipendiat Kristina Strasunskiene Senior Research Scientist Kalman Nagy, SINTEF Professor Emeritus Knut Schrøder Stipendiat Silje Skogvold
Lorentzen, Marianne Supervisor: Examiners:	Stereoselektiv syntese av optisk aktive, umettede aminer og alkoholer fra sulfinylforbindelser. Associate Professor Odd Reidar Gautun Associate Professor Bård Helge Hoff Associate Professor Tore Lejon, UiT
Lystvet, Sina Maria Supervisors: Examiners:	Kjemo-enzymatisk syntese av enantiomert rene 2-haloalkoholer. Studier av disse som substrater for lipasene CALA og CALB. Associate Professor Bård Helge Hoff Professor Emeritus Thorleif Anthonsen Associate Professor Eirik Sundby, HiST Professor Torbjørn Ljones
Martinsen, Morten Supervisor: Examiners:	Utvikling og uttesting av automatisert målesystem for Beinlim i kobber elektrolytt. Professor Øyvind Mikkelsen Senior Research Scientist Kalman Nagy, SINTEF Stipendiat Silje Skogvold
Martinsen, Thomas Supervisors: Examiners:	Innvirkning av redusert forurensning på sporelementer i jord og planter på Sørlandet. Professor Eiliv Steinnes Professor Torunn Berg Associate Professor Elin Gjengedal, UMB Chief Engineer Bjørn Ove Berthelsen, Trondheim kommune Associate Professor Trond Peder Flaten

## Post Graduate Students

Møllegård, Ståle	$\beta$ -metylamino-L-alanin [BMAA], en av nevrotoksisk aminosyre, i blod, hjernevev og lever hos pasienter med amyotrofisk lateralsklerose og parkinsonisme-demens fra stillehavsøya Guam.
Supervisors:	Associate Professor Trond Peder Flaten Associate Professor Per Bruheim
Examiners:	Professor Lars Skjeldal, UMB Professor Torbjørn Ljones
Neerland, Elisabeth	Utvikling av analytisk metode for automatiske målinger av viktige spormetaller i kystvann.
Supervisors:	Professor Øyvind Mikkelsen Stipendiat Kristina Strasunskiene
Examiners:	Senior Research Scientist Kalman Nagy, SINTEF Professor Knut Schrøder
Salomonsen, Silje Naper	Delegering av miljøansvar fra stat til kommune. En case-studie av kommunal iverksetting av forurensningsforskriftens kapittel 2 om opprydding i forurenset grunn ved bygge-og gravearbeider.
Supervisors:	Adjunct Professor Rolf Tore Ottesen Chief Engineer Marianne Langedal, Trondheim kommune
Examiners:	Research scientist Sissel Holvik, NIBR Chief Engineer Bjørn Ove Berthelsen, Trondheim kommune Associate Professor Rudolf Schmid
Skårn, Jenny Skeide	Kilder for polysykliske aromatiske hydrokarboner (PAH) i jord i Oslo, Norway.
Supervisors:	Adjunct Professor Rolf Tore Ottesen Professor Jan Alexander, The Norwegian Institute of Public Health
Examiners:	Chief Engineer Bjørn Ove Berthelsen, Trondheim kommune Associate Professor Rudolf Schmid
Sørensen, Kari Bjerke	Structural investigations on the hydrolysis of molybdenum oxomethoxide.
Supervisors:	Dr. Pablo Beato, Topsøe A/S, Denmark Professor David Nicholson
Examiners:	Research Scientist Bjørnar Arstad, SINTEF, Oslo Post.doc. Merete Hellner Nilsen, UiO Associate Professor Morten Bjørgen

## MSc in Environmental toxicology and chemistry 2008

Holsen, Aase Marie Hersleth	Sporelementer i bjørn og ulv i Norge: En landsomfattende undersøkelse.
Supervisors:	Associate Professor Trond Peder Flaten Senior Research Scientist Hans Christian Pedersen, NINA Professor Eiliv Steinnes
Examiners:	Chief Technician Syverin Lierhagen Senior Research Scientist John Atle Kålås, NINA Professor Torunn Berg

## Master project, exchange students

Ausin Reguera, Maider	Impact of NOM on trace metal speciation. Studies of copper levels and complexing capacity in river water using combination of different analytical techniques.
Supervisor:	Professor Øyvind Mikkelsen
Examiners:	Professor emeritus Knut Schrøder Stipendiat Silje Marie Skogvold
Corcóstegui Ruiz-Carrillo, Cecilia	Impact of NOM on trace metal speciation. Quantification of trace metals including mercury in rivers in catchment areas correlated against quantity of NOM and type of vegetation.
Supervisor:	Professor Øyvind Mikkelsen
Examiners:	Professor emeritus Knut Schrøder Stipendiat Silje Marie Skogvold



## MSc in Chemistry/Siv.ing. 2008

Dahl, Espen Hvidsten Supervisor: Cosupervisor: Examiner:	Hydraulic permeability of fluoridic solutions in Nation Professor Signe Kjelstrup Research Scientist Thor Anders Aarhaug, SINTEF Research Manager Ann Mari Svensson, SINTEF
Høgmoen, Hanne Supervisor: Examiner:	Synthesis of polyfluorinated tertiary amines with potential antifungal activity Associate Professor Bård Helge Hoff Quality Assurance Manager Viggo Waagen, Borregaard Synthesis AS
Lervik, Anders Supervisor: Cosupervisor: Examiner:	Energy dissipation in biomolecular motors Professor Signe Kjelstrup Associate Professor Fernando Bresme, Imperial College London Professor Bjørn Kvamme, UiB
Melnes, Silje Supervisor: Examiner:	Asymmetric catalytic aziridination of alkenes for the purpose of manufacturing substituted 2-aminotetralines Associate Professor Odd Reidar Gautun Associate Professor Tore Hansen, UiO

## MSc in Education, Chemistry

<b>Bjørk, Tine Beate</b> Supervisor: Examiner:	<b>Syntese av crocin-derivater.</b> Professor Vassilia Partali Associate Professor Birte Sjursnes, HiØ Dr.ing. Eva Mørkved
<b>Brimi, Aslak Opsahl</b> Supervisor: Examiner:	<b>Likevekt i læring, læring i likevekt? En studie av kjemisk likevekt i forhold til undervisning.</b> Professor Lise Kvittingen Stipendiat Per-Odd Eggen Associate Professor Vivi Ringnes, UiO Associate Professor Annette Lykknes
<b>Elgen, Marianne</b> Supervisor: Examiner:	<b>Fremstilling og karakterisering av potensielle virkestoffer mot sopp og protozoer.</b> Associate Professor Bård Helge Hoff Associate Professor Birte Sjursnes, HiØ Professor Torbjørn Ljones
<b>Frøland, Stine Lindset</b> Supervisor: Examiner:	<b>Barns kjemiske lekemiljø. Nivå og kilder til PAH i barnehagejord i Trondheim.</b> Adjunct Professor Rolf Tore Ottesen Divisional Engineer Lise Støver, Trondheim Kommune Chief Engineer Bjørn Ove Berthelsen, Trondheim kommune Associate Professor Rudolf Schmid
<b>Hansen, Mari Roen</b> Supervisor: Examiner:	<b>Likevekt i læring, læring i likevekt? En studie av kjemisk likevekt i forhold til undervisning.</b> Professor Lise Kvittingen Stipendiat Per-Odd Eggen Associate Professor Vivi Ringnes, UiO Associate Professor Annette Lykknes
<b>Hole, Marianne Prestvik</b> Supervisor: Examiner:	<b>Miljøgifter i barns lekemiljø.</b> Adjunct Professor Rolf Tore Ottesen, Divisional engineer Lise Støver, Trondheim Kommune Chief Engineer Bjørn Ove Berthelsen, Trondheim kommune Associate Professor Rudolf Schmid

**Valved, Hilde**

Supervisor:

Examiner:

**Atmosfærisk kvikksølvspesiering i Ny-Ålesund. Hvor pålitelig er den nåværende metoden?**

Professor Torunn Berg  
Stipendiat Anne Orderdalen Steen  
Research Scientist Katrine Aspmo, NILU  
Associate Professor Florinel G. Banica

**PhD in Chemistry**

Boman, Mats Henrik Linus

Trial lecture

Supervisor

Evaluation committee

Cholesky decomposition based methods in electronic structure theory.  
Exchange-correlation density functionals – present status.  
Professor Henrik Koch  
Professor Jeppe Olsen, Aarhus University, Denmark  
Professor Trygve Ulf Helgaker, University of Oslo, Norway  
Professor Per-Olof Åstrand Department of Chemistry, NTNU

Gellein, Kristin

Trial lecture

Supervisor

Co-supervisors

Evaluation committee

High resolution inductively coupled plasma mass spectrometry: Some applications in biomedicine.  
Mulige helseeffekter relatert til utslipp av metaller til luft.  
Associate Professor Trond Peder Flaten  
Professor Eiliv Steinnes, Department of Chemistry  
Professor Tore Syversen, Department of Neuroscience  
Professor Gunnar Nordberg, Occupational and Environmental Medicine, Umeå University, Sweden  
Senior Scientist Hilde Thelle Uggerud, Norwegian Institute for Air Research, Kjeller, Norway  
Professor Torunn Berg, Department of Chemistry, NTNU

Ingebrigtsen, Stian

Trial lecture

Supervisor

Evaluation committee

The influence of chemical composition on streamer initiation and propagation in dielectric liquids.  
Ageing and breakdown of HV solid insulating materials stressed by ns, HV transients.  
Professor Per-Olof Åstrand  
Professor Steven A. Boggs, Institute of Materials Science, University of Connecticut, USA  
PhD Leif A. A. Petterson, ABB Corporate Research, Sweden  
Professor Hans Kristian Høidalen, Department of Electric Power Engineering, NTNU

Inzoli, Isabella

Trial lecture

Supervisor

Evaluation committee

Coupled transports of heat and mass at the surface of and inside silicalite. Snowflakes.  
Professor Signe Kjelstrup  
Associate Professor dr. Thijs Vlugt, Delft University of Technology, The Netherlands  
Professor dr.ing. Dag Dysthe, Department of Physics, University of Oslo, Norway  
Associate Professor Morten Bjørgen, Department of Chemistry, NTNU

Jartun, Morten

Trial lecture

Supervisor

Co-supervisor:

Evaluation committee

Active sources and dispersion mechanisms of pollutants, especially polychlorinated biphenyls (PCBs), in the urban environment.  
Making sense of pollutant levels: Moving from chemical analysis to risk assessment of their significance and potential risk management.  
Professor Eiliv Steinnes  
Adjunct Professor Rolf Tore Ottesen, NGU, Norway  
Professor Kevin C. Jones, Department of Environmental Science, Lancaster University, UK  
Professor Gijs D. Breedveld, Department of Environmental Engineering, Norwegian Geotechnical Institute, Oslo, Norway  
Professor Torunn Berg, Department of Chemistry, NTNU

## Post Graduate Students

Nordhei, Camilla	Aspects of electronic and structural properties of nanophase cubic ferrites studied by X-ray absorption spectroscopy. Including the decomposition of carbon dioxide over hydrogen-reduced ferrites.
Trial lecture	Reduced emissions by conversion of carbon dioxide.
Supervisor	Professor Astrid Lund Ramstad
Evaluation committee	Professor Wendy Flavell, School of Physics and Astronomy, University of Manchester, UK Dr. Nina Aas, StatoilHydro, Trondheim, Norway Professor Magnus Rønning, Department of Chemical Engineering, NTNU
Svendsen, Monica L.	A study of metal contamination in a natural ecosystem affected by smelter emissions.
Trial lecture	Determination of metal bioavailability and exposure in the environment.
Supervisor	Professor Eiliv Steinnes
Co-supervisor	Hans Andreas Blom, Østfold University College, Sarpsborg, Norway
Evaluation committee	Associate Professor John R. M. Derome, Rovaniemi research Station, Finnish Forest Research Institute, Finland Associate Professor Elin Gjengedal, Department of Plant and Environmental Sciences, Norwegian University of Life Sciences, Norway Professor Torunn Berg, Department of Chemistry, NTNU
Yu, Qiang	Synthesis of optically active nucleosides, nucleotides and oligonucleotide analogues.
Trial lecture	Diversity-oriented organic synthesis: Concepts, applications and limitations.
Supervisor	Professor Per Carlsen
Evaluation committee	Professor Mikael Begtrup, Department of Medicinal Chemistry, University of Copenhagen, Denmark Associate Professor Anette Bayer, Department of Chemistry, University of Tromsø, Norway Associate Professor Odd Reidar Gautun, Department of Chemistry, NTNU

## Student Exchange from NTNU, Department of Chemistry 2008

Name	Specialization	Level	Institution
Egede-Nissen, Cecilie	MKJ-Analyt.chem.	MSc, 4th yr	Vrije Universiteit Brussel, Belgium
Grave, Anlaug Haukvik	MKJ-Struct.chem.	MSc, 5th yr	University of Newcastle, Australia
Høgmoen, Hanne	MTKJ-Org.chem.	MSc, 5th yr	University of California, Berkeley, USA
Høyvik, Ida-Marie	BKJ-Struct.chem.	BSc, 3th yr	University of California, Berkeley, USA
Lervik, Anders	MTKJ-Phys.chem.	MSc, 5th yr	University of London, UK
Lyngvi, Eirik	MTKJ-Org.chem.	MSc, 4th yr	University of California, Berkeley, USA
Sørum, Christopher	MTKJ-Org.chem.	MSc, 4th yr	University of California, Berkeley, USA
Valvik, Beate	MKJ-Struct.chem.	MSc, 5th yr	University of Newcastle, Australia
Åstrand, Ove Alexander	MTKJ-Org.chem.	MSc, 4th yr	University of California, Berkeley, USA

## Student exchange to NTNU, Department of Chemistry 2008

Name	Institution
Akyalcin, Sema	Anadolu University, Eskisehir, Turkey
Breukers, Stefanie	RWTH, Aachen, Germany
Cabana, Beatriz Louriño	Universidad de la Coruña, Spain
Corcostegui, Cecilia	University of the Basque Country, Spain
Hocke, Nils	Georg-August-Universität Göttingen, Germany
Kalz, Kai	Georg-August-Universität Göttingen, Germany
Lüttschwager, Nils	Georg-August-Universität Göttingen, Germany
Martin, Daniel	RWTH, Aachen, Germany
Paul, Jean-Nicolas	Université des Sciences et Technologies, Lille, France
Reguera, Maider Ausin	University of the Basque Country, Spain

Staff

## Academic Staff

### Organic Chemistry



Group Leader  
Professor, Dr.ing.  
Anne Fiksdahl



Adjunct Professor, Ph.D.  
(Oxford). Derek Chadwick



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



Professor, Ph.D. (Buffalo).  
Per Carlsen



Associate Professor, Dr.ing.  
Odd Reidar Gautun



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



Associate Professor, Dr.scient  
Bård Helge Hoff



## Physical Chemistry



Group Leader  
Associate Professor, Dr.scient.  
Astrid Lund Ramstad



Assistant Professor  
Terje Bruvoll



Professor, Dr.philos.  
Reidar Stølevik



Professor, Dr.scient.  
Bjørn Alsberg



Professor, Dr.techn.  
Signe Kjelstrup



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



Adjunct Professor, Dr.philos.  
(Utrecht). Dick Bedeaux



Professor, Ph.D. (Århus).  
Henrik Koch



Associate Professor, Ph.d.  
Morten Bjørgen



Professor, Ph.D. (Madison)  
Torbjørn Ljones

**Environmental and Analytical Chemistry**



Group Leader  
Dr.Scient  
Øyvind Mikkelsen



Professor, Dr.scient.  
Lise Kvittingen



Professor, Dr.philos.  
Eiliv Steinnes



Associate Professor, Dr.ing.  
Florinel G. Banica



Ph.D.  
Karina Mathisen



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



Professor, Dr.scient.  
Torunn Berg



Professor, Ph.D. (London)  
David Nicholson



Associate Professor, Ph.D.  
Annette Lykknes



Associate Professor, Dr.ing.  
Trond Peder Flaten



Adjunct Professor  
Rolf Tore Ottesen

### Administrative staff



Head of administration  
Anne Langseth



Senior Executive Officer  
Lillian Hanssen



First Secretary  
Aase Sæther



Executive Officer  
Inger Marie Frøseth



Higher Executive Officer  
Ingrid Kristine Tømmerdal

### Technical staff



Staff Engineer  
Stein Almo



Head Engineer  
Julie Jackson



Staff Engineer  
Nina Klausen



## Staff



Head Engineer  
Syverin Lierhagen



Senior Engineer  
Tron Rolfsen



Engineer  
Kari Tanem



Engineer  
Kjersti Ljones



Staff Engineer  
Gunnar Svare



Staff Engineer  
Roger Aarvik

## Scientific Assistants

Angelsen, Ragnhild Strand  
Braaten, Hans Fredrik  
Burheim, Odne S.  
Engøy, Ingemund F.  
Gebremariam, Kidane Fanta  
Holt, Yngvil  
Kong, Xiang Yi  
Lervik, Anders  
Lie, Aleksander  
Melnes, Silje  
Nordløyken, Marit  
Sandru, Eugenia-Mariana  
Siegesmund, Øyvind  
Skorpa, Ragnhild  
Steen, Anne O.  
Tvedt, Thor Håkon Krane  
Øvergård, Tommy

## Demonstrators

Berg, Michel Brunet  
Bergesen, Amund Dolva  
Braaten, Hans Fredrik  
Delic, Asmira  
Edvardsen, Tove-Nanny  
Eliassen, Ragnhild  
Gunby, Anders Sværi  
Helgerud, Trygve  
Holsæter, Hege  
Holt, Yngvil  
Høiås, Morten  
Jacobsen, Julie B.  
Karlsen, Tom Rune  
Kjønstad, Ingrid Fadum  
Kristiansen, Tina  
Kaasa, Kristin  
Landsem, Eva  
Lian, Nikolai  
Lieungh, Ida  
Lyngvi, Eirik



## Demonstrators contd.

Martinsen, Morten	Smørvik, Marte Songøygard
Næss, Mari Kirkebøen	Solvang, Tina
Ohm, Ragnhild	Sundrønning, Silje Beate
Ringholm, Magnus	Særslund, Anne Lene
Selsaas, Eirik	Takla, Marit
Siegesmund, Øyvind	Tungen, Jørn E.
Sivertsen, Ida Karoline	Vestrum, Magnus Inderberg
Skarra, Ragne Marie	Volynkin, Andrey S.
Skorpa, Ragnhild	Vågenes, Birgitte Bårli
Skråmo, Silje	Willassen, Veronica
Skårn, Jenny Skeide	Yttervik, Johan Hatling
Slinde, Gøril Aasen	Aardal, Eivind

## Guest professors/researchers/lecturers

Krzysztof Rokosz	Feb. 11 – 14, 2008
Gabriel Billon	Feb. 11 – 15 and Nov. 24 - 28, 2008
Marine Nalbandyan	June 23 – 30, 2008
Donald L. Macalady	June 30 – July 28, 2008
Jon Pharoah	July 21 – Dec. 31, 2008
Daniel Barragan	Sept. 11 – Dec. 28, 2008
Brigitte Van Tiggelen	Sept. 17 – 23, 2008
Irina Shtangeeva	Oct. 14 – Nov. 27, 2008
Levent Akyalcin	Oct. 15 – Dec. 31, 2008
Professor Emil Palecek, Institute of Biophysics, Academy of Sciences of the Czech Republic, Brno, Czech Republik: "Electrochemistry of nucleic acids and proteins. New Trends in protein analysis"	Aug. 19, 2008
Professor Vladimir Vetterl, Centre of Biophysics, Masaryk University and Institute of Biophysics, Academy of Sciences of the Czech Republic, Brno, Czech Republic: "Self-assembled layers of nucleic acid components and Oligodeoxynucleotides at the electrodes"	Aug. 19, 2008
Dr. Brigitte Van Tiggelen, Université Catholique de Louvain, Belgium "Closing a Chemical Controversy from the Periphery: J.B. Van Mons and the reduction of calx of mercury"	Sept. 23, 2008
Professor Daniel Barragán, Chemistry Department, Universidad Nacional de Colombia, Bogotá, Colombia: "Instabilities in non-equilibrium systems"	Oct. 21, 2008
Dr. Sudipto Muhuri, University of Barcelona, Spain: "Role of molecular motor kinetics in collective vesicular Transport and structural stability in biofilaments"	Oct. 28, 2008
Professor Steven Boggs, University of Connecticut, USA: "Theory for the worst case tolerable conducting defect (particle) in transmission class solid dielectric cables"	Nov. 6, 2008
Dr. Irina Shtangeeva, St. Petersburg University, Russia: "Neutron activation analysis in determination of trace And ultra trace elements in biological material"	Nov. 24, 2008



# Annual Report for Department of Chemistry 2008



## **NTNU - Innovation and Creativity**

The Norwegian University of Science and Technology (NTNU) in Trondheim represents academic eminence in technology and the natural sciences as well as in other academic disciplines ranging from the social sciences, the arts, medicine, architecture to fine arts. Cross-disciplinary cooperation results in ideas no one else has thought of, and creative solutions that change our daily lives.

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