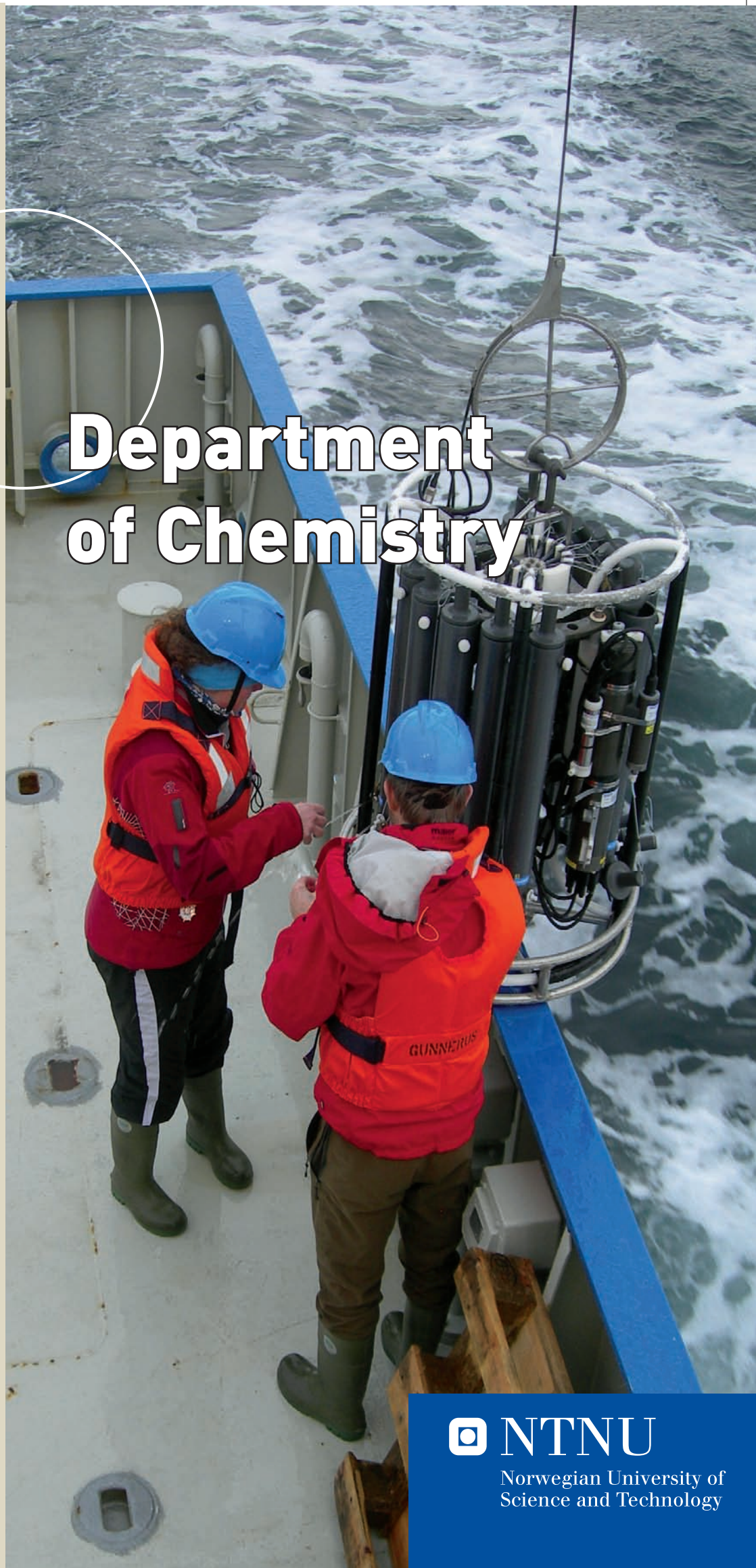


Annual Report 2009

Department of Chemistry



 NTNU

Norwegian University of
Science and Technology

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COVER PAGE

Onboard NTNU's research vessel, R/V Gunnerus, collecting samples of seawater from the Trondheim fjord

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The State of the Department of Chemistry 2009

Introduction

The global economic climate in 2008 was characterised by a feeling of gloom and doom. By contrast, during 2009 there were encouraging signs that made us cautiously optimistic. We have started the process of scrutinising the Research Council of Norway's evaluation of Norwegian chemistry departments. One step in response was to create a Committee of the Future (CoF) with a broad mandate to look into all aspects relating to the Department and to report to the Head of Department in March 2010. This process is linked to the Department's work on the new Strategic Plan for the period 2010 – 2014.

CoF consists of three scientists with leadership experience, all chemists but from different NTNU departments: Professor Tor Grande (Department of Materials Science and Engineering), Professor Sigurd Skogestad (Department of Chemical Engineering) and Professor Eiliv Steinnes (Department of Chemistry). Professor Grande is Chairman.

Measures to increase income

This is a perennial item in my report and I remain impressed by the activities and productivity of some of our researchers who are still working under trying circumstances. Of the above mentioned chemistry departments, the main role of the Department of Chemistry is to take care of basic or curiosity-driven research. We are therefore guided by a strategy that includes working towards increased external funding additional to that from a cash-strapped Research Council.

This has given, for example, results in the form of a Statoil-funded collaboration us and partner Canadian universities. The topic is environmental impact studies on the enormous oil sand deposits in that country.

We are also working with SINTEF and others on an application for an SFI (Centre for Research and Innovation) project that will be submitted to the Research Council in 2010.

Statoil is collaborating with us on another environmental project by financing an adjunct professorship which was advertised in the latter half of 2009; the result of which will be announced early in 2010.

The Swiss-Norwegian Beamlines

at the European Synchrotron Radiation Facility, Grenoble.

This is a consortium that was proposed and founded 20 years ago by the Department together with the Department of Physics. Today, the Norwegian members of the consortium are NTNU, Institute for Energy Technology, University of Oslo, University of Stavanger, University of Tromsø, and the Research Council of Norway. The Swiss partners are ETH, Zürich, University of Lausanne, University of Berne, the University of Geneva and the Swiss Office for Education and Research. From 1st June 2009 the Chairman of the consortium is Prof David G. Nicholson of this Department.

A considerable part of the Department's research activity is directed towards the SNBL and seven MSc students completed their course of study in which synchrotron radiation played the major role in their research topics.

The Department is also active in the planning of two beamlines at the proposed new synchrotron (Max IV) at MaxLab in Lund, Sweden.

Mass Spectrometry Consortium

Since we have extensive interests in mass spectrometry we took the initiative to invite in the first instance the Department of Biotechnology to collaborate with us in starting up a collaboration within this field. The initiative has expanded both in ambition and number of partners, for example SINTEF. The Department of Biology has expressed interest as well.

The Strategic Plan 2010 – 2014

The process, which will culminate in the new Strategic Plan, started with a programme of weekly discussions in the autumn of 2009. The results will be input to the Strategy Seminar to be held in March 2010 at Jægtvold Hotel.

*David G. Nicholson
Head of Department*

The Fluoro-organic group: Chiral compounds with potent antifungal activity¹

Treatment of an increasing number of infections associated with immuno-compromised patients is causing a marked increase in the number of fungal strains showing resistance to presently available antimycotic agents.^{2,3} Among others, *Cryptococcosis*, caused by members of the *Cryptococcus neoformans* species, is a serious and potentially fatal fungal disease afflicting a large number of AIDS patients.⁴ Two groups of chiral amines structurally related to Butenafine (**1a**) and Terbinafine (**2a**) have been synthesised and tested as potential antifungal agents.

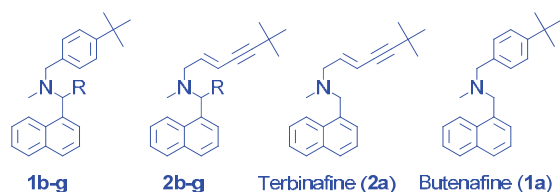
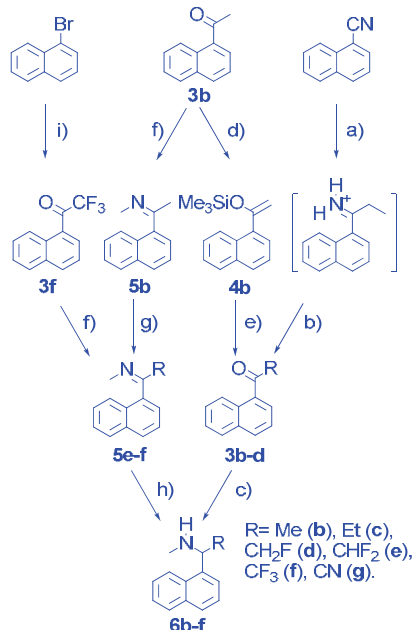


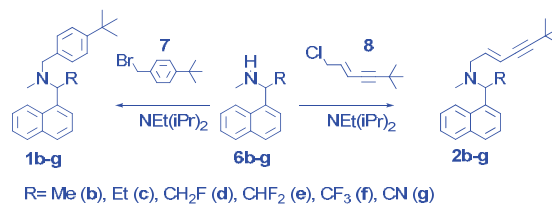
Figure 1. The structures Butenafine (**1a**), Terbinafine (**2a**) and the studied compounds **1b-g** and **2b-g**, R = Me (**b**), Et (**c**), CH₂F (**d**), CHF₂ (**e**), CF₃ (**f**), CN (**g**).

Synthesis

The key building blocks, **6b-f**, were synthesised by different methods as shown in Scheme 1.



Scheme 1: Synthetic methods for preparation of **6b-f**: a) EtMgBr/THF; b) H⁺/H₂O, c) NH₂Me, AcOH, NaBH₃CN; d) LiHMDS, TMS-Cl; e) F-TEDA-BF₄; f) NH₂Me, TiCl₄ g) NFSI, mol. sieve, K₂CO₃; h) NaBH₃CN, AcOH; i) Ethyl trifluoroacetate



Scheme 2: Synthesis of *rac*-**1b-g** and *rac*-**2b-g**.

Biological testing

Testing of antifungal activity was performed in the group of Colin Charnock (HIO). The derivatives **2b-g** were all less active than Terbinafine (**2a**) towards *C. neoformans*. More interesting results were obtained for **1b-g** (Table 1)

Comp.	R	Calc. pKa	Rel. size	MIC ₅₀ (g/mL)	MIC ₇₅ (g/mL)
Butenafine (1a)	H	9.2	0	0.125	0.25
<i>Rac</i> - 1b	Me	9.5	0.52	0.125	0.25
<i>(R)</i> - 1b	Me	9.5	0.52	<0.031	0.031
<i>(S)</i> - 1b	Me	9.5	0.52	0.5 ^[c]	1.8 ^[c]
<i>Rac</i> - 1c	Et	9.8	0.56	0.25-4 ^[c]	8
<i>Rac</i> - 1d	CH ₂ F	7.9	0.62	>16	>16
<i>Rac</i> - 1e	CHF ₂	6.1	0.68	>16	>16
<i>Rac</i> - 1f	CF ₃	3.2	0.91	>16	>16
<i>Rac</i> - 1g	CN	5.4	0.40	>16	>16

^[c]Trailing growth complicated assignment of MIC values.

Table 1: Antifungal activity (MIC) of **1a-g** towards *C. neoformans*

The activity of the compounds depended on the stereochemistry, the size and the electronic properties of the substituents. Enantiopure (*R*)-**1b** was found to be 4 times more active than Butenafine (**1a**) towards *C. neoformans*, and also performed better towards, *C. diffluens* and *T. cutaneum*. This suggests that antimycotics based on this compound might be an improvement of existing Butenafine-based formulations. Structure activity studies are currently ongoing using (*R*)-**1b** as a new lead compound.

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Bård Helge Hoff and Erik Fuglseth

Research Projects

Theoretical modelling of interfacial transport.

There are many natural phenomena and industrial processes which involve heat and mass transfer. As soon as there is a difference in temperatures between two places, heat goes from the hot to the cold one. Similarly, if there is a difference in the amount of some substance, it starts to flow from the place with higher concentration to the place with lower one. These are the essence of the Fourier and Fick's law established long ago. They were first established as experimental laws, but later found naturally in the theory of non-equilibrium thermodynamics [1]. This theory gives a systematic way to describe transport phenomena without needing the details of a particular system.

A class of interesting systems are surfaces. From a macroscopic point of view they are the interfaces between two different phases, like between gas and liquid or between two immiscible liquids. These phases have essentially different physical properties, and what happens in between these phases is very interesting. A common way to describe the interface is to consider it as a spatial region where the properties change continuously from one phase to the other. Of course, this behaviour is different from what happens in either of the phases. From a macroscopic point of view the surface is sharp, and whatever changes therefore must change within a very short distance, typically a few nanometers. The drastic changes of physical properties over a very short region are described by introducing the gradients of densities as variables, in addition to the densities themselves. This theory is known under several names, particularly, the square gradient theory, the diffuse-interface model, the H-model, etc. In equilibrium it gives the main coexistence properties between two phases, in particular it gives the surface tension.

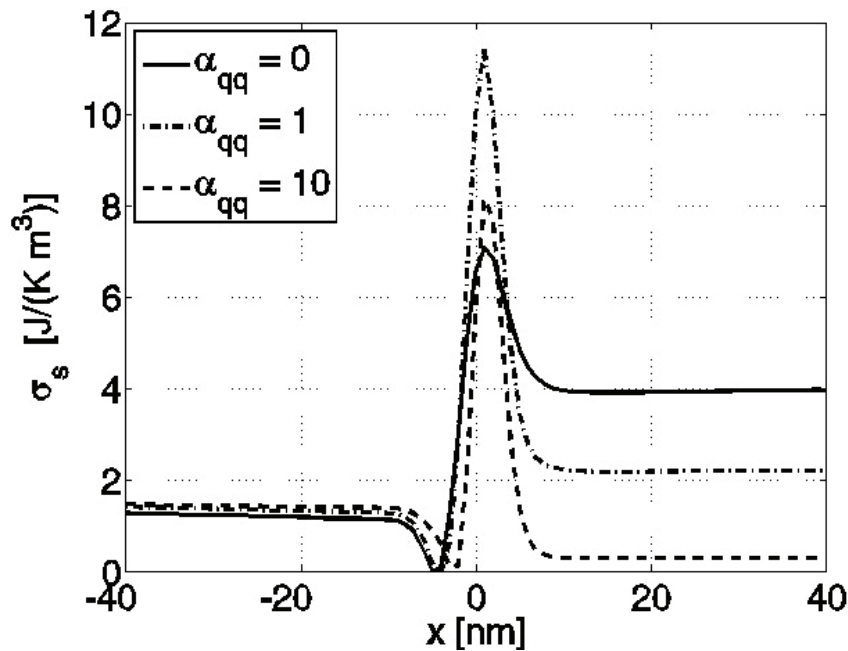
In many relevant applications there is heat and mass transfer through the interface. Among others, one could think of distillation, osmotic phenomena, biological transport in cells. It is therefore important to describe these phenomena properly. We combined the general theory of non-equilibrium thermodynamics with the square gradient model of the interface in order to do that. As a result we get a non-equilibrium description of the interface. Applying the developed theory, we can confirm the assumptions used to build macroscopic thermodynamics of the surface [2], as well as to get

the practical predictions of transport coefficients for industry.

We divided the work in three different stages. First, we developed a general framework to study the transport properties of the surface. Second, the theoretical description allowed us to understand particular factors which affect the interfacial transport. Finally, we were able to give some numerical estimates of measurable quantities, which can be verified in practice and give feedback to the model assumptions. The research was the subject of a PhD-programme and is presented in the papers [3-6].

A non-equilibrium description, as described in [1], requires input from two big areas: thermodynamics and hydrodynamics. A connection between them is the relation between rates of change of thermodynamic quantities, namely the Gibbs relation. It comes as postulate in any non-equilibrium description: comparing the experiments with predictions of a theory can prove or disprove a particular assumption. The common method in the description of the homogeneous phase is to assume that the equilibrium Gibbs relation is also valid in non-equilibrium. In the interfacial region this assumption is not as transparent as in the bulk: abrupt changes of the order parameter affects the rate of change of thermodynamic quantities. We postulated a modified Gibbs relation to be used in the non-equilibrium of the surface which lead to a consistent theory.

The key quantity in the non-equilibrium thermodynamics is the entropy production. It shows how fast the entropy density changes and is a measure of the irreversibility of the process. In equilibrium it is zero, while in non-equilibrium processes it is always positive, according to the second law of thermodynamics. In the general theory [1,2] the entropy production can be split into a sum of several terms, which have a different origin but a similar structure. All these terms are found to be products of a thermodynamic force and a thermodynamic flux. The use of a non-conventional Gibbs relation allows us to obtain an expression for the entropy production inside the interfacial region which has exactly this form. This in turn gives the insight on the nature of the thermodynamic forces and fluxes in the surface.



Entropy production profile for a binary mixture which is being evaporated after a 5% decrease of the pressure in the gas. The values of the parameters α give the amplitude of the heat resistivity peak in the interfacial region.

The drastic change of the fluid density through the surface lead to a similar behaviour of other quantities. One of the quantities which has an observable effect is the enthalpy density. The difference of the enthalpies between liquid and vapour is the enthalpy of vaporization, which shows how much energy one needs to supply to liquid in order to evaporate it. We have shown that this difference is relevant for the transport properties of the surface. Moreover, we found that not only this difference is an important quantity. The whole enthalpy profile across the interfacial region plays an important role for the value of the resistivities for transport through the surface.

Finally, we were able to give some numerical prediction of the transport properties of the surface. There are different theories which are used to do that, results of which can be compared to the results of our work. One of these theories is kinetic theory, which assumes the molecules in the fluid to be hard spheres. It is good for the description of gases but not applicable for liquids. We have shown that it underestimates the values of some transfer properties of the interfacial region, which means that the influence of liquid is important for the surface.

Furthermore, our method contains a number of adjustable parameters which come as an input. Values of these parameters are found from experiments and may be used for different conditions. In this way we can test our theory and give particular advises for industry.

Concluding, the developed theory opens a wide range of further research. Studying different components at various conditions we can cover different industrial needs. Moreover, further theoretical analysis is needed to study different phenomena.

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K.S. Glavatskiy and D. Bedeaux

Research Projects

Porcine Pancreatic Lipase (PPL), important for drug synthesis and Cystic Fibrosis treatment

From Trondheim to Barcelona

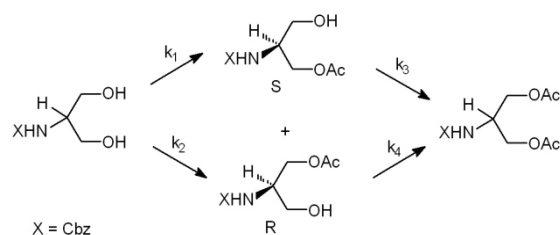
The Spanish-Norwegian cooperation was initiated in 2006, when master student Marte Marie Hansen Frigstad in the Biocatalysis group, spent a one year research period at Instituto de Quimica Avanzada de Catalunya in Barcelona, under the supervision of professors Pere Clapes and Jesús Joglar. The group of Clapes and Joglar participated in the EU cooperation "Applied Biocatalysis" led by professor Thorleif Anthonsen, and happened to be perfect hosts for Marte, both scientifically and socially!



Right: Pere Clapes, Jesús Joglar and Elisabeth Jacobsen discussing iminocyclitol synthesis during a coffee break at Biotrans in Bern in July 2009. Left: Marte Frigstad stayed at home with her new born daughter, however, the contact between Marte and her spanish "boy-friends" is still very good!

Chiral iminocyclitols

By asymmetric acetylation of prochiral Cbz-2-amino-1,3-propanediol with vinyl acetate and Porcine Pancreas Lipase (PPL, Sigma Type II Crude Steapsin, L3126) in THF (Scheme 1), Marte was aiming to synthesise enantiopure synthons for conversion into iminocyclitols as potential anti-infective agents due to inhibition of bacterial glycosyl transferases and glucosidases.



Scheme 1

The two-step desymmetrisation process outlined in Scheme 1 is virtually a one-step process, because no achiral diacetate was observed. A mixture of R and S monoacetates were produced.

Enantiomeric excess (ee) changes during reaction

It is usually anticipated that the ee of a desymmetrisation is constant during reaction. However, Marte observed that the ee of the product ester changed during the reaction (measured by chiral HPLC). After prolonged reaction, the predominant configuration of the product changed from the S-enantiomer to the R-enantiomer! (Figure 1) Observations of similar reaction systems based on measurement of enantioselectivity at one single point of conversion, do not reveal changes in ee. Our results clearly demonstrates the importance of monitoring the progress of the reaction.

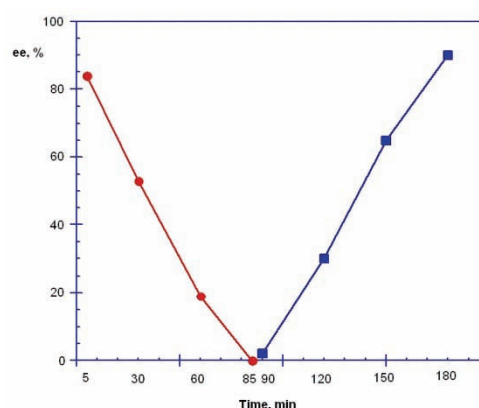


Figure 1. Desymmetrisation of Cbz-2-amino-1,3-propanediol by PPL catalysed acetylation. (S)-Monoacetate (red), (R)-monoacetate (blue).

Isoenzymes of PPL Desymmetrisation

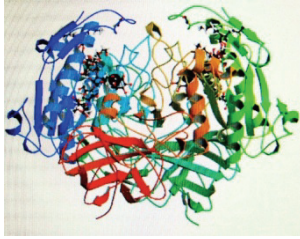
Aleksander Lie (M. Sc. 2009) continued the project after Marte finished her M. Sc. in 2007. By use of different PPL preparations in esterification of Cbz-2-amino-1,3-propanediol, Aleksander found that the changing ee of the product was due to the action of two lipases (isozymes) with opposite stereoselectivity.

Purified PPL Sigma Type VI-S, L0382 in THF with vinyl acetate as acyl donor, gave only the S-enantiomer. Moreover, when vinyl acetate acted both as solvent and acyl donor together with crude PPL, only the R-enantiomer was produced.²

Sigma-Aldrich joins the project

In 2009, Sigma-Aldrich (Switzerland) joined the project. Head of Specialites Research, Dr. Roland Wohlgenuth, found the Norwegian investigations of the widely used Sigma-Aldrich PPL preparations, to be of great importance for the company. Dr. Elisabeth Jacobsen (Dept. of Chemistry, HIST, Trondheim) and professor Thorleif Anthonsen presented the important and surprising results at Biotrans 2009 in Bern, Switzerland in July. Wohlgenuth, and also Clapes and Joglar, as well as 500 other academic and industry researchers from all over the world were present.

PPL widely used



Enzyme extracts from the porcine pancreas is regarded as a "grandfather drug" used for many years as treatment of persons suffering from pancreas dysfunctions and malnutrition, amongst them 70 000 Cystic Fibrosis (CF) patients worldwide.

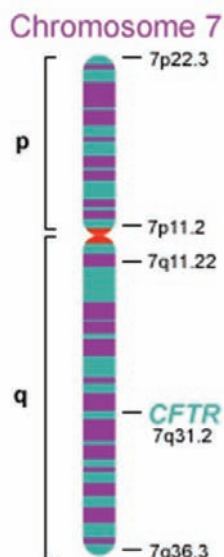
PPL is also used in large amounts as catalyst in production of several fine chemicals and pharmaceuticals (by DSM, Lonza, Sigma-Aldrich etc.), f. inst. in glycidol and cyclopropanediol synthesis.³



Thorleif Anthonen, Roland Wohlgemuth and Norwegian speaking Ludger Wessjohann from Leibniz Institute of Plant Biochemistry, (Halle, Germany) discussing enzymatic C-C coupling by prenylation, which was the theme of Wessjohann's lecture. (Wessjohann has been a visiting scientist at University of Oslo with professor Lars Skattebøl).

FDA regulation of Cystic fibrosis PPL.

In 2004, the American Food and Drug Administration (FDA) decided to set the "grandfather drug" under investigation, securing correct amount of active ingredients and correct dosing for the CF patients.⁴ CF is a genetic disease caused by mutations in a gene located on chromosome 7, which directs the epithelial cells of the body to produce a defective form of a protein called cystic fibrosis transmembrane conductance regulator (CFTR). The protein product of the defective gene causes the body to produce unusually thick,



sticky mucus that clogs the lungs and leads to life-threatening lung infections, obstructs the pancreas and stops natural enzymes from helping the body break down and absorb food. Creon (PPL from Solvay Pharmaceuticals) is the only treatment approved by FDA for this purpose, however it is still under investigation. Benedicte Abello (15) from Barcelona, living in Lillehammer, suffers from Cystic fibrosis. She has been taking Creon before every meal all her life. Fortunately, she is healthy and is now a coming ice dancer.



Knowledge Based Bio-Economy (KBBE) in EU FP 7

The European bio-economy, which focuses on sustainable management, production and use of biological resources, through life sciences and biotechnology, has an approximate market size of over €1.5 trillion, comprising more than 22 million people. Within this, White Biotechnology (biocatalysis), is estimated to have a market size around €100-160 million by 2010.⁵ Several 2010 EU FP 7 calls deal with the use and search for new enzyme catalysts.

OECD is now regarding White Biotechnology as a sustainable and green method of large importance in the conversion of fossil fuel into fine chemicals and bio-energy.

In Norway, Aker BioMarine, Pronova BioPharma, GC Rieber Oil, Borregaard Synthesis etc. use enzyme technology in their production of fine chemicals and pharmaceuticals.

1. Marte M. H. Frigstad, M. Sc. NTNU 2007
2. Aleksander Lie, M. Sc. NTNU 2009
3. Roland Wohlgemuth, personal communication
4. <http://www.cff.org/treatments/Therapies/Nutrition/Enzymes>
5. www.mckinsey.com/clientservice/.../pdf/biovision_booklet_final.pdf

Torbjørn Ljones
Thorleif Anthonen

Research Projects

Book project:

Academy and industry – 100 years of chemistry training in Trondheim

In 2010 NTNU, Norway's only technical university celebrates its centenary. From 1910, the Norwegian Institute of Technology (NTH) was able to offer chemical engineering education in what was referred to as the "best furnished and best equipped chemical laboratory in Scandinavia." A research project dealing with the history of the chemistry education in Trondheim throughout the past 100 years, has been initiated. The study will culminate in a book to be published by an academic publisher.

The project covers the history of chemical training in Trondheim starting from its establishment at NTH in 1910 until today, through periods which saw growth and crisis, two world wars, expansion in the 1950s, the establishment of a department of chemistry at the Norwegian College of Teaching in Trondheim (NLHT) in 1960, education explosion, oil and information ages, and finally a merger of the chemistry milieus into NTNU in 1996.

The chemical institutions, including their students, professors, departments and research will, not surprisingly, serve as the main actors. However, the university did not exist in isolation, thus its history must be seen within a societal context as well. The project aims at understanding the role of NTNU in relation to the international history of chemistry and the history of Norwegian industry. The history of the chemistry departments at NTNU reflects the multiplicity of chemistry; from process chemistry to nano chemistry, from organic and inorganic chemistry to wood processing, seaweed research, environmental chemistry etc. The interaction between the technical, industrial oriented culture and the scientific university culture is one of the distinctive features of the history of chemistry education at NTNU.

Funding

The project has received funding from NTNU (Faculty of Natural Science and Technology, Department of Chemistry, Department of Chemical Engineering, Department of Materials Science and Engineering, Department of Biotechnology), as well as from private sponsors (SINTEF Materials and Chemistry, Sør-Norge Aluminium, XStrata Nickel, StatoilHydro, Södra Cell Tofte, Treforedlingsindustriens bransjeforening, Stiftelsen Papirindustriens Forskningsinstitutt).

Editorial committee

The project was initiated by Lise Kvittingen, Anne Kristine Børresen and Annette Lykknes. The editorial committee consists of nine members representing different areas of chemistry as well as the history of science:

Joakim Ziegler Gusland, Historian, Department of Chemistry (main author)

Annette Lykknes, Associate professor, Department of Chemistry (project leader and co-author)

Lise Kvittingen, Professor, Department of Chemistry
Torbjørn Helle, Professor emeritus, Department of Chemical Engineering

Sigurd Skogestad, Professor, Department of Chemical Engineering

Jomar Thonstad, Professor emeritus, Department of Materials Science and Engineering

Anne Kristine Børresen, Professor, Department of History and Classical Studies

Jan Thomas Kobberød, post. doc., Department of History and Classical Studies

Mentz Indergaard, Senior Advisor, Information Division



A chemistry laboratory at NTH

Annette Lykknes

Force-field models for molecular properties

Force fields are normally used in molecular dynamics and Monte Carlo simulations for the calculation of interatomic and intermolecular interactions. Since the energy of the system and the forces between all the particles have to be calculated repeatedly (simulations are carried out on the time-scale of nanoseconds whereas the integrator take time-steps in the order of a femtosecond), a force field should be based on very simplified expressions for the molecular energy. Consequently, a force field is not as sophisticated as accurate quantum chemical calculations, but it is anyway required that it includes the essence of the chemistry of the molecules.

In a force field, the energy is divided into different energy terms, each described by set of atom-type parameters. The intramolecular energy are often divided into bond stretches, angle bending and torsional motion, whereas the intermolecular energy terms (also used for long-range intramolecular energies) are normally divided into electrostatic, polarization and van der Waals (short-range repulsion and dispersion) terms.

Recently, we have focused on accurate models for the electrostatics and the polarization. The electrostatic energy is normally calculated with Coulomb's law by using atomic charges, sometimes extended by atomic dipole and quadrupole moments. To obtain accurate atomic charges is by no means trivial. For example, atomic charges are not transferable in the sense that e.g. carbon charges, q_C are the same everywhere. Instead, an atomic charge depends on the chemical surroundings, for example q_C in a C=O group is highly positive whereas q_C in C-H has a small negative value. A common method to actually model this behaviour is the electronegativity equalization model (EEM), where each atom type is described by an electronegativity and a chemical hardness. Thus the difference in atomic electronegativity, ξ_J between two atoms determines the direction of the charge transfer between the atoms, and since $\xi_H < \xi_C < \xi_O$, the correct behaviour of the carbon charges discussed above is obtained. However, in the EEM, the atomic charges have to be calculated in each time step of the simulation by solving a set of linearly coupled equations, which leads to substantially increased computational time in molecular dynamics simulations.

One way to include electronic polarization is to use atomic polarizabilities as atom-type parameters and again use classical electrostatics. The electric field from the surrounding atoms (described by e.g. atomic charges) induces an atomic dipole moment that in turn gives an additional electric field on the neighbouring atoms. So also the polarization gives a set of linearly coupled equations that needs to be solved in each time-step during the simulation.

Since 2000, we have developed a polarization model based on the point-dipole interaction (PDI) model (reviewed in [3]). Briefly, the PDI model is

based on the classical interaction of a set of isotropic point polarizabilities interacting with each other in an external electric field, where the atom-type polarizabilities are parametrized to mimic the molecular polarizability. The model development has resulted in a number of studies of polarization in large molecular systems, primarily on carbon nanotubes and fullerenes (see figures 1 and 2), but also boron nitride tubes and proteins (see figure 3) have been studied. For the tubes and fullerenes, the main objective has been to study the scaling of the polarizability with the size of the system and it has been demonstrated that the present model can serve as a bridge between molecular and macroscopic properties. For proteins, the model gives useful information about the local dielectric constant.

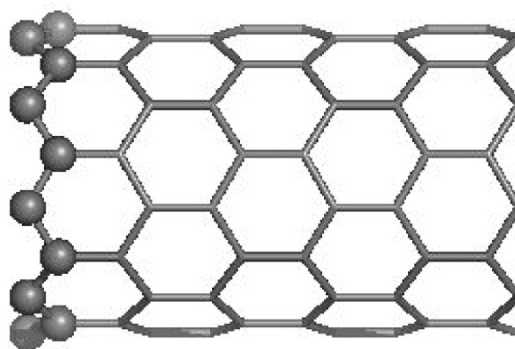


Figure 1. A [9,0] carbon nanotube. A segment of 108 atoms is shown.

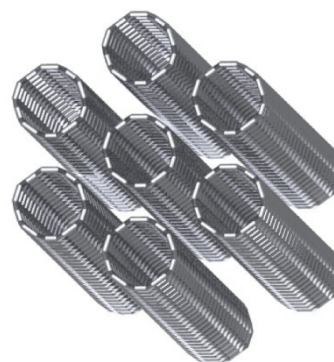


Figure 2. A nanotube rope. The extent of shielding of the polarization of the inner tube has been studied.

Subsequently, the EEM and PDI models have been combined into one model where thus charge-transfer terms also contribute to the polarizability (see for example [2]). However, the EEM has a fundamental problem in the sense that it is a "metallic" model, i.e. there is not any resistance for charge-transfer along a molecular chain. Consequently, the molecular polarizability for the combined EEM/PDI model does not scale correctly for example with the length of a nanotube. We have therefore developed a new model, a combined charge-transfer and PDI model (CT/PDI) where an extra energy term has been added for charge

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transfer between two atoms through a third atom [4]. Thus, a resistance for charge transport along a molecular chain has been included. A simple test of the model was to study the dipole moment of both alkanes and polyenes both connected to an aldehyde group at the end of the chain (see figure 4). The required behaviour was obtained, i.e. that the dipole moment of the alkane chain is almost constant with the length of the chain whereas the charge-transfer terms dominate for the polyenes. For the polyenes, the dipole moment is therefore increasing with the length of the molecule as charge is transferred along the chain (see figure 5)

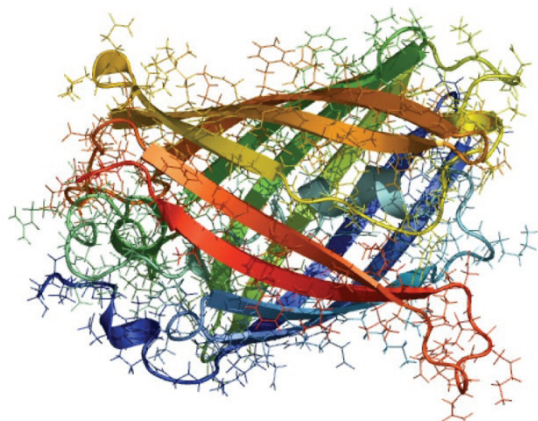


Figure 3. Green fluorescent protein (GFP). The dielectric response has been calculated in this protein amongst others.

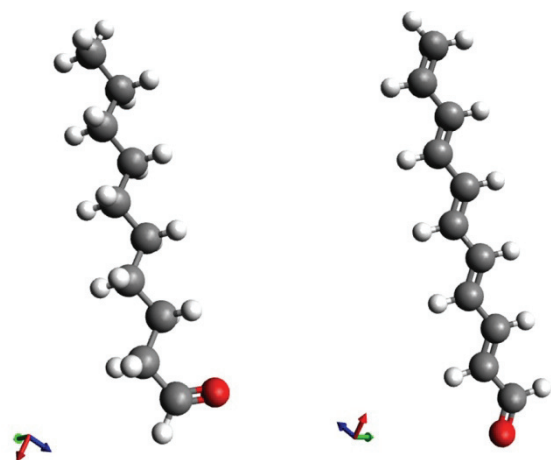


Figure 4. Alkane (left) and polyene (right) with a terminating aldehyde group. The purpose is to have two systems with completely different charge-transfer contributions.

The model has also been extended to the frequency-dependent polarizability [1, 5], which gives opportunities to calculate non-linear optical properties of molecular materials and to extend the method to molecular electronics. The basic idea is to assign a time-dependence for the oscillating atomic charges and atomic dipole moments and thereby to obtain expressions for the kinetic energy. Then the Lagrangian is minimized for the kinetic and potential energy using standard techniques. So far the model has only been established, and it has been demonstrated that alkanes, polyenes and

aromatic systems can be described with the same set of atom-type parameters although their frequency-dependence are quite different.

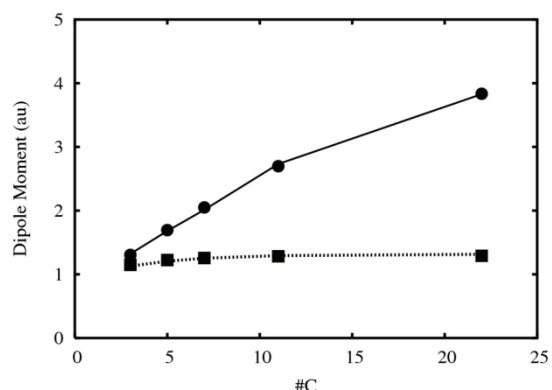


Figure 5. The dipole as a function of the number of carbon atoms in an alkanal chain (bottom) and polyenal chain (top). The points represent DFT data and the lines represent our model showing the excellent agreement.

There is a manifold of prospects for the method. The goal is to include it as the molecular mechanics part of a combined quantum mechanical and molecular mechanics (QM/MM) model and to include it as the electrostatic energy in a reactive force field. The method itself is developed to also give local dielectric constants, infrared and Raman intensities, molecular conductivity, and Fukui indices to describe reactivity in molecules.

Per-Olof Åstrand

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RESULTS FROM THE LABORATORY OF RENEWABLE ENERGY

NTNU is since long engaged to promote research for energy and environmental concerns. One contribution from the Department of chemistry to this area is an active fuel cell laboratory. Other contributions are studies of energy efficient operation in industry. Irreversible thermodynamics gives the theoretical basis for experiments and applied activities related to fuel cells, hydrogen storage, salt power plants, thermoelectric generators, and heat integration in industrial equipment. These activities are core activities within the field of Renewable Energy.

In 2009, two doctor degrees were obtained within this field. The first thesis "Transport on a nanoscale; quasi-elastic neutron scattering and molecular dynamics studies" [1] dealt with mechanism of hydrogen transport to the electro catalytic site. Some results from the second thesis, "Thermal effects in polymer electrolyte fuel cells" [2] are highlighted below.

Thermal effects in PEM fuel cells

The effort worldwide to commercialise fuel cells is very large. Materials must be cheaper and energy efficiencies higher, in order to make this power producer viable. Our group works on the thermal signature of the polymer electrolyte fuel cell (PEMFC), as a measure of its efficiency, as one of few groups. This was the main motivation for constructing an apparatus that allows us to measure 1) the thermal conductivity of fuel cell components and their thermal contact resistivities and 2) the energy dissipated as heat during fuel conversion, leading to the PhD degree of Odne Burheim on the 26th of November 2009.

The thermal conductivity apparatus is presented in Figure 1. The material thickness is measured at a given compaction pressure, enabling us to report new data [2]-[4]. Thermal conductivities are needed in the modelling thermal effects within the PEMFC. [5]-[6]

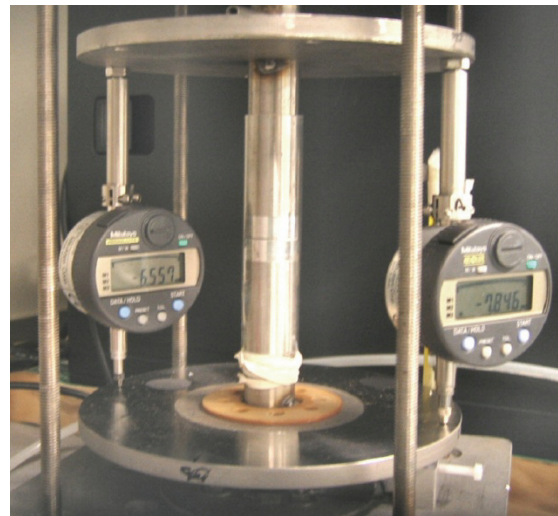
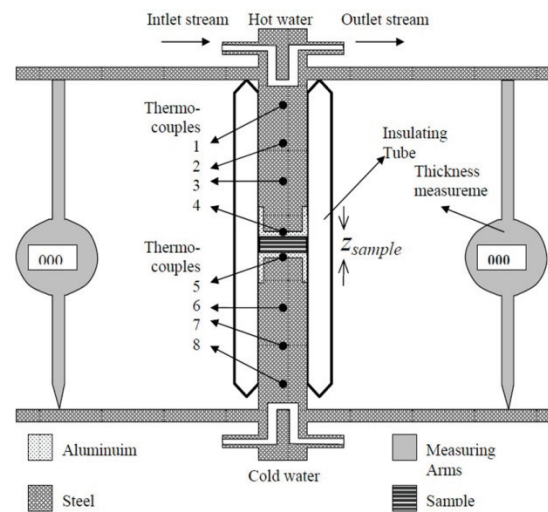


Figure 1. A sketch (top) and a picture taken in the laboratory of the thermal conductivity apparatus.

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The constructed calorimeter was tailored around a PEM single fuel cell. This apparatus is new. By combining measurements of heat and work produced from the fuel cell at constant temperature and pressure, we report a possible new mechanism for energy loss in the cell, by in situ hydrogen peroxide formation [7]. A sketch of the apparatus along with a picture taken in the lab is shown in Figure 2.

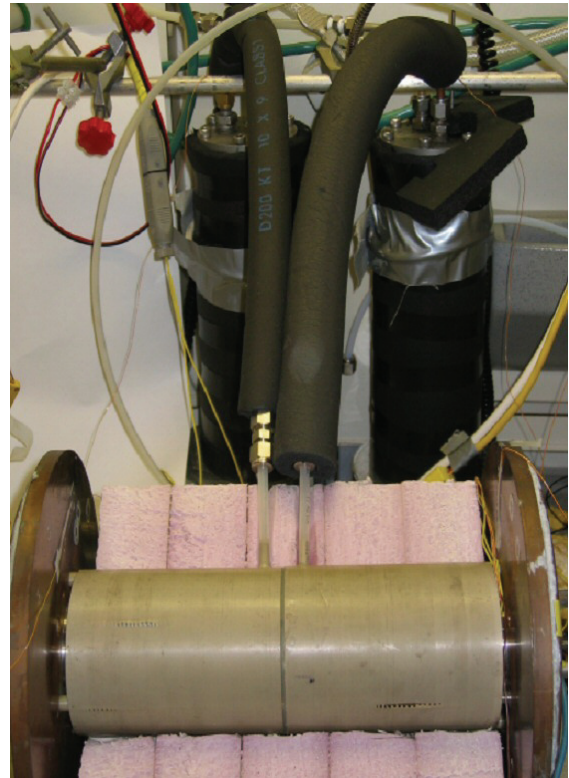
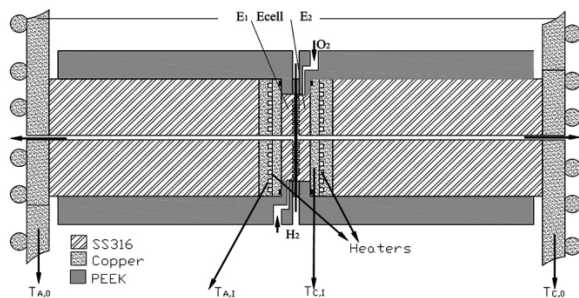


Figure 2. A sketch (left) and a picture taken in the laboratory of the fuel cell calorimeter.

Two senior guest scientists spent their sabbatical in this laboratory in 2009, Ass. Professor Dr. Jon Pharoah and Dr. Levent Akyalcin. Dr. Pharoah contributed to the thesis work [2]. Dr. Akyalcin measured thermal osmosis effects in fuel cell components. Two exchange students on the master level, Hannah Lampert and Maria Lohse visited from German universities. Lampert measured thermal conductivities of porous transport layers. Lohse measured the Seebeck effect of cells with identical electrodes.

Thermoelectric power generation

The Norwegian metallurgical industry generates waste heat at relatively high temperatures, up to 800 C. With the present concern about energy efficiency, a project is started to study how this waste heat can be useful. The conversion between thermal and electric energy makes use of the

Seebeck effect and takes place in a so called thermoelectric convertor. It has so far been calculated [8] that the heat emitted from casting of ferro silicon can be used to operate fans that clear the atmosphere in the casting area.

Reverse electro dialysis

At the beginning of 2010, with a new grant from NFR, FRIENERGI [9], we can establish a laboratory to develop reverse electro dialysis salt power plant technology. In this plant, the salt in the seawater is reversibly transported via ion-exchange membranes into river water. The current is then collected at the end from the ferric/ferrous red ox reaction. [10] This is illustrated in Figure 3. The project includes a post.doc. (Dr Burheim) a PhD (to start summer 2011) and Ass. Professor Dr. J. Pharoah, Queens University, Ontario, Canada. This project is meant to last for approximately five years.

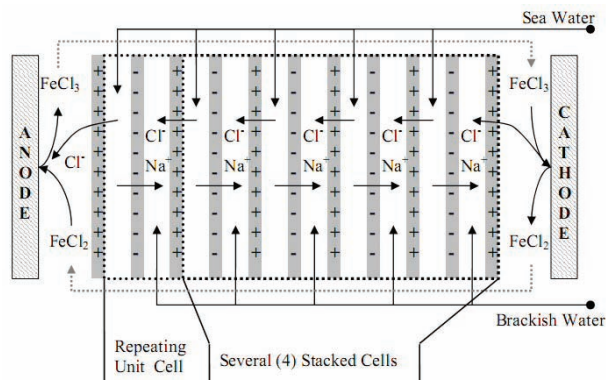


Figure 3. Sketch of the system planned to harvest DC power by mixing brackish and sea water. The electrode materials serve as electron acceptors for the red-ox reactions in the anode and the cathode compartments. Transports of anions and cations in the appropriate ion exchange membranes are indicated.

Entropy Production Minimisation in the Industry

What you save, is what you earn! By being more energy efficient, resources are spared and hopefully also with profit as energy prices are increasing. Entropy production is thus a highly useful term, as it defines and pinpoints lost potential work in a process. Extraction of work from waste heat in the industry relates to this by recovering parts of the entropy produced.

Several studies are made in our group on how to map and improve the energy efficiencies in processes. Together with Statoil Dr. Stip. Mari Voldsund is mapping the entropy production of an off-shore production rig in the North Sea. In collaboration with Air Liquide and Sintef Energy research Dr. Stip. Leen van der Ham is working on energy efficiency cryogenic air separation as a part of the 7th Framework program "DECARBit". This programme aims to demonstrate pre-combustion CO₂ capture within at a reasonable cost.

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Odne Burheim and Signe Kjelstrup

Research Projects

Understanding the mechanisms of chemical evolution: Writing the history of High Performance Liquid Chromatography (HPLC)

History of chemistry is the key bridging discipline between the practice of chemistry and the humanities, concerning itself with the recording, description and interpretation of the evolution of chemistry through time as well as with the educational, social, institutional, political, economical and technological contexts of this evolution.

In September 2009, a PhD project in the history of the HPLC was initiated. This research project is targeting the history of the chromatographical techniques, focusing at the major evolutionary steps of liquid chromatography during the decades exactly after the Second World War. Filling a gap in the current historiography of chromatography, this project will help to the construction of a handy case study usable on a number of different issues related to the science-technology and industry relations, economical and policy drives for research and innovation, teaching of chemistry, and bridging of disciplines on a theoretical and practical level through common research practices and methods.

From its very beginning chromatography has been an interdisciplinary method both at its roots and its applications. The initial method was developed during the first years of the 20th century by Mikhail Tswett (1872-1919), a botanist with a physical chemical approach towards physiology. During the mid-World War years it grew to become a major tool of general analytical chemistry, pivotal to the development of fields such as biochemistry, petroleum chemistry and –after the 1950s— genetics.

Our research will use the creation of the first HPLC prototype in 1968-69 by the group of Csaba Horváth (1930-2004) at the laboratories of Yale University as the point of gravity, to aim both backwards and forwards in time. Backwards, the process, theoretical and technological, from the older gas chromatography apparatus to HPLC will be mapped and reconstructed through archive material and original publications and placed into the broader context of the era, while forwards, an unravelling of the rather complicated progress of the method out of the academia and into the mass production lines and R&D labs of multinationals will be attempted. Archive work at Yale University Library and at the Chemical Heritage Foundation will be conducted in order to investigate the development of later chromatographical techniques in America.

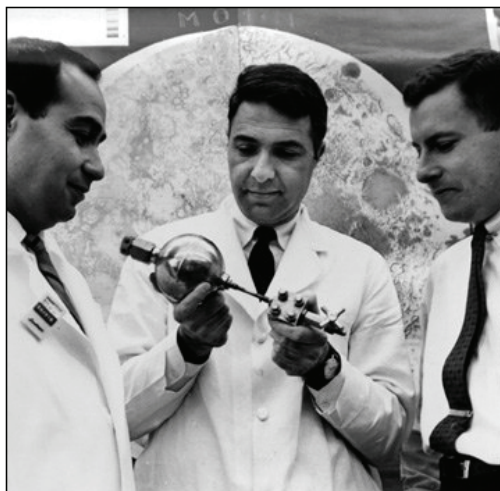


Fig. 1: Dr. Lipsky (center) of Yale University holds a lunar GC component in 1962. The lunar GC was part of the overall Apollo project, developed as a method for analysing the later expected "Moon Rocks".

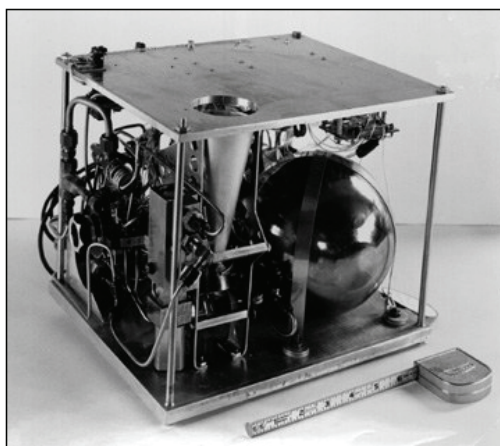


Fig. 2: The lunar GC.

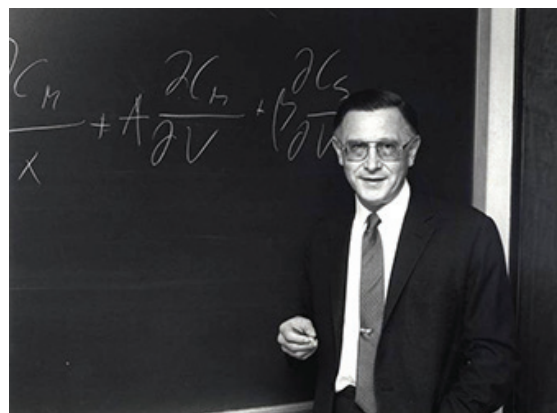


Fig. 3: Csaba Horváth, the builder of the first HPLC.

Apostolos Gerontas and Annette Lykknes

Workshop, Non-Equilibrium Thermodynamics



On 27 August 2009 Signe Kjelstrup became 60 years old. Helped by the support of the Institutt for Kjemi we were able to organise a two day International Workshop with the title "Non-Equilibrium Thermodynamics" on the 3rd and the 4th of September. The Dekan of the Science Faculty, Prof. Dr. Bjørn Hafskjold opened the workshop and gave a presentation highlighting her career and the importance and relevance of her work. A distinguished international group of speakers (2 Japan, Saudi Arabia, 2 Spain, USA, UK, Canada, Netherlands, 2 Norway) had accepted our invitation to give a presentation.

The workshop had 54 participants and was generally considered to be a great success. The level of the contributions was outstanding and led to interesting discussions about the latest developments in the field. For the (MSc, PhD) students attending it was a very inspiring experience.

On behalf of the organising committee, we would like to convey our appreciations for your kind financial support for the event, making it possible to cover travel, expenses and accommodations for the invited speakers.

Focus and Scope of the Workshop: Over many years Signe Kjelstrup has been pioneering the foundation and the application of non-equilibrium thermodynamics. Regarding the fundamentals she contributed to the verification of local equilibrium, the development of mesoscopic thermodynamics to describe active transport and the extension of non-equilibrium thermodynamics to transport into and through surfaces. The theory has over the years actively been verified by applying it to electrochemical cells, membrane systems as well as for distillation columns by entropy production minimization. Effort has also been made to the use of non-equilibrium molecular dynamics to study these systems on a molecular level. The validity of the Onsager relations in homogeneous phases as well as for surfaces was verified in this manner. The workshop reviewed the highlights of the development of irreversible thermodynamics by discussing both theoretical and applied aspects in an international context with leading scientists in the field.

Organising committee:

Dick Bedeaux, NTNU, Trondheim, Norway.
 Terje Bruvoll, NTNU, Trondheim, Norway.
 Torleif Holt, SINTEF, Trondheim, Norway.
 Steffen Møller-Holst, SINTEF, Trondheim, Norway.
 Preben Vie, IFE, Kjeller, Norway.

Dick Bedeaux

Activities

“NTH 1910” – Student Exhibition in the Natural Science Library

In 2006, the course RFEL3093, Episodes in the history of science, was launched as an option for students at master level at the Faculty of natural sciences and technology. Each year, the students are assigned course work and we encourage the use of the historical collections at Department of chemistry and Department of physics, which are well kept and contain gems of scientific instruments from 100 years of research and teaching at NTNU. This year, as we were drawing close to the centenary of the university, the students were asked to make an exhibition for the natural science library under the heading “NTNU 100 years”, exploring, amongst other things, some of the objects collected from the previous 100 years. Each student, individually or in pairs, wrote an essay about the history and local context of an instrument, or another topic connected to the chosen theme of the exhibition.

Topics explored and displayed this year were “Trondheim – the city of knowledge”, “Development of industry around 1900 and its impact on the demand for engineers”, “Students at NTH 1910-20”, “Science around 1910 – as seen through the journal *Naturen*”, “The refractometer”, “Electrometers in physics through history – teaching and research”, “Crookes tube” and “Coulomb’s torsion balance” – all within the context of NTH (the Norwegian Institute of Technology) 1910. In addition, assignments from previous students on the spectrophotometer as well as on the Daniell cell were studied in order to display these instruments and present aspects of their history.

The students made an effort to prepare an informative and at the same time aesthetically satisfying exhibition, shedding light on the 100 years of teaching and research in chemistry and physics at NTNU. The students involved were Frode Aalmen, Tove-Nanny Edvardsen, Solvor Motland Evensen, Stian Hagli, Marit Anne Holten, Sigrid Iversen, Vegard Ovesen, Astrid Toftaker Rise, Kirsti Rø and Ragnhild Skorpa. Previous work by Per-Odd Eggen, Martin Riber and Magnus Mellingsæter was included as well.



Some of the scientific objects on display



The students responsible for the exhibition: Vegard Ovesen (back left), Astrid Toftaker Rise, Solvor Motland Evensen, Tove-Nanny Edvardsen, Ragnhild Skorpa, Frode Aalmen, Stian Hagli, Kirsti Rø (front left) and Marit Anne Holten. Sigrid Iversen was not present.

Annette Lykknes

Kjemiløypa 2009 – The Chemistry Trail 2009

The chemistry trail at NTNU was organized for the first time in March 2009 and provided an opportunity for 12-year olds to experience and learn chemistry through curriculum-based experiments.

2005 was the International Year of Physics, for which the Department of Physics and the Resource Centre for Mathematics, Science and Technology Education at NTNU created the physics trail. They aimed to provoke curiosity and stimulate wonder at how nature works. The physics trail was popular to the extent that it became an annual event for 6th grade school children. During the autumn semester 2007, the biology trail was organized for 9th graders and has been equally successful. The chemistry education group at the Department of Chemistry was challenged to contribute a chemistry trail. This was realised after several rounds of fund raising, logistics and development of a scientific programme. Our aim has been to stimulate both senses and intellect by providing scientific experiments that schools normally cannot offer their pupils.

700 school children

More than twice as many schools registered for the chemistry trail as our capacity allowed, so unfortunately many were turned down. A total of 24 primary schools in North and South Trøndelag counties were welcomed, and in a period of two weeks around 700 children visited the Department of Chemistry at NTNU. Between 9.30 a.m. and 2.00 p.m. the pupils, accompanied by their teachers and escorted by university students, were taken from point to point in laboratories and seminar rooms of the Natural Science Building at Gløshaugen.



The iodine clock reaction



Gas production and detection using small, portable laboratories

The programme was directed at 7th graders and the experiments adapted to their curriculum; thus the pupils could have fun and yet learn relevant chemistry. We wanted the students to get their own, hands-on experiences in chemistry; therefore they conducted most of the experiments themselves.



Experiments with dry ice

Amongst other things, the children tested stones for iron, "smoked" cigarettes through cotton using a water aspirator, experimented with dry ice and liquid nitrogen, watched colour reactions and experienced heat exchange in chemical reactions. In some of the experiments the students encountered small, portable laboratories which have been developed for schools in South Africa.



Making slush using liquid nitrogen

Activities

The response was enormous. 654 of the around 700 participants filled in an evaluation form; of these, 91% were very satisfied. Typically the pupils replied that it was “fun” and that they hoped they would return. Moreover, they were very pleased with the university students who escorted and supervised them. When asked whether or not the chemistry trail encouraged them to want to learn more science, 63% responded positively. To what extent this will have long-term results remains to be seen, however many children showed enthusiasm and excitement. As one of them expressed it: “I knew nothing before, everything I know I learnt today, and I do not know what more there is to learn.”



The children are being welcomed by university student Hans Fredrik Veiteberg Braaten

17 university students employed

17 student assistants were employed during the chemistry trail 2009. They alternated between being responsible for conducting the experiments in one specific room, and taking a group of students from point to point. During the two weeks every student assistant had tried all tasks. In order to ensure security, the students had to undertake two days of training, led by Per-Odd Eggen who was in charge of the scientific programme. The experience the student assistants acquired from the chemistry trail must be considered a bonus. After some days of running-in they improved the chemistry trail considerably and stood as competent leaders and enthusiastic scientists. Project leaders were Lise Kvittingen and Annette Lykknes, who, amongst other things, took care of the fund raising, logistics, as well as the acquiring and preparing equipment and chemicals – which is not a small task considering the many reagents and quite large volumes, e.g. around 100 L of starch solution for the iodine clock reaction. The positive feedback from the school children, teachers and university student assistants is certainly inspiring for further development of the chemistry trail.



Student assistants under training

Funding and assistance

The chemistry trail was funded by NTNU, Tekna and South Trøndelag County, which together contributed some 300.000 NOK. Without this support, offering a scientifically solid and secure programme would not have been possible. Many thanks! We are also indebted to Inger Frøseth, Roger Aarvik and Gunnar Svare for their practical assistance, without which the chemistry trail would never have become reality.

Per-Odd Eggen, Lise Kvittingen and Annette Lykknes

Photos: Per-Odd Eggen, Ingrid Fadum Kjønsstad, Annette Lykknes, Marit Nordløyken and Silje Skogvold.

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Steinnes, Eiliv.

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An old fishing vessel at the pier

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Organic Chemistry

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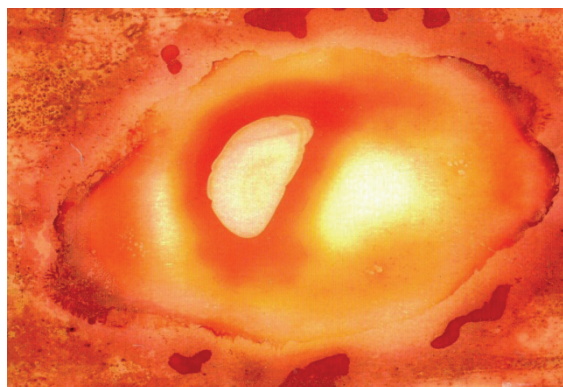
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Esmurziev, Aslan; Sundby, Eirik; Hoff, Bård Helge. Regioselective C-6 Hydrolysis of Methyl O-Benzoyl-pyranosides Catalysed by Candida Rugosa Lipase. *European Journal of Organic Chemistry* 2009; vol. 10. p. 1592-1597

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Activities

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Physical Chemistry

Bedeaux, Dick.

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NTNU

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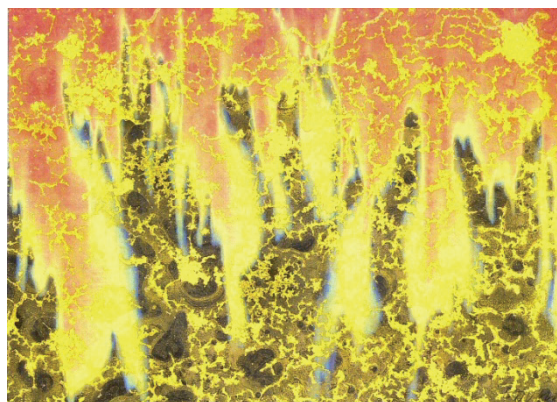
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Kjelstrup, Signe.

Non-Equilibrium Structures:How can they be maintained?. I: Confluence. Interdisciplinary Communications 2007/2008. Oslo: Centre for Advanced Study at the Norwegian Academy of Science and Letters 2009 ISBN 978-82-996367-6-6. p. 85-89

Kjelstrup, Signe.

Tørketid. Forskningspolitikk 2009 (4) p. 5-5

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In situ XAS and IR studies on Cu:SAPO-5 and Cu:SAPO-11: the contributory role of monomeric linear copper(I) species in the selective catalytic reduction of NO_x by propene. Physical Chemistry, Chemical Physics - PCCP 2009; vol. 11 (26) p. 5476-5488

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Decomposition of Carbon Dioxide at 500°C over Reduced Iron, Cobalt, Nickel and Zinc Ferrites: A Combined XANES-XRD Study.. The Journal of Physical Chemistry C 2009; vol. 113(45) p. 19568-19577

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Nonequilibrium thermodynamics of transport through moving interfaces with application to bubble growth and collapse. Physical Review E. Statistical, Nonlinear, and Soft Matter Physics 2009; vol. 80(2) p. -

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The molecular structure of gaseous 1,2 cyclohexanedione. Journal of Molecular Structure 2009 ; vol. 923 (1-3) p. 94-97

Smalø, Hans Sverre; Ingebrigtsen, Stian; Åstrand, Per Olof.

Calculation of Ionization Potentials and Electron Affinities for Molecules Relevant for Streamer Initiation and Propagation. IEEE transactions on dielectrics and electrical insulation 2009

Smalø, Hans Sverre; Åstrand, Per-Olof; Jensen, Lasse.

Nonmetallic electronegativity equalization and point-dipole interaction model including exchange interactions for molecular dipole moments and polarizabilities. Journal of Chemical Physics 2009; vol. 131(4)

Sparta, Manuel; Høyvik, Ida-Marie; Toffoli, Daniele; Christiansen, Ove.

Potential Energy Surfaces for Vibrational Structure Calculations from a Multiresolution Adaptive Density-Guided Approach: Implementation and Test Calculations. Journal of Physical Chemistry A 2009; vol. 113(30) p. 8712-8723

van der Ham, LV; Gross, J; Verkooijen, A; Kjelstrup, Signe.

Efficient Conversion of Thermal Energy into Hydrogen: Comparing Two Methods to Reduce Exergy Losses in a Sulfuric Acid Decomposition Reactor. Industrial & Engineering Chemistry Research 2009; vol. 48(18) p. 8500-8507

Activities

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

B. Alsberg

Section Leader, Physical Chemistry Group, Department of Chemistry, NTNU, Sep. 1 – Dec. 31, 2009.

11th Scandinavian Symposium on Chemometrics (SSC), Loen, Norway, June 8 – 11, 2009.

Co-author on Lecture on: Validation of Molecular Structures Sampled by Evolutionary Algorithms Using an Intuitive Screening Model.

Researcher's Night, NTNU, Trondheim, Sep. 25 - 26, 2009.

Lecture on: Hyperspektral-kamera med projektor - gjør det usynlige synlig.

CSI Trondheim, Researcher's Night, NTNU, Trondheim, Sep. 25 - 26, 2009.

Lecture on: Hyperspektralt kamera og projektor: Å gjøre det usynlige synlig.

T. Anthonsen

Scientific Board Member: European Federation of Biotechnology, Section for Applied Biocatalysis, ESAB.

Conference "24. Organisk kjemisk vintermøte", Skeikampen, Norway, Jan. 8 – 11, 2009.

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

Management Committee Meeting "Cascade Chemoenzymatic Processes – New Synergies between Chemistry and Biochemistry", Bruxelles, Belgium, May 26, 2009.

Conference "Biotrans 2009", Bern, Switzerland, July 5 – 10, 2009.

Co-author on Poster Presentation: Lipase Selectivity in Resolutions and Asymmetrisations. Allosteric Effects.

Science Week 2009, Minneapolis, USA, Sep. 27 – 30, 2009.

Invited Speaker. Lecture on: A European Model for Transatlantic Cooperation in Science.

Seminar at Aalborg University, Denmark, Dec. 15, 2009.

Co-Author on Lecture on: Enantioselectivity in Lipase Catalyzed Resolutions and Symmetrisations Changes during Reaction. Important also for Non-Enzymatic Reactions?

Aalborg University, Denmark, Dec. 16, 2009.
1st Opponent Doctoral Thesis Defence of Sinthuwat Ritthitham.

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.

Member of Organizing Committee of the Summer School "Nanomaterials in Biomedical Sciences", Bratislava, Slovak Republic, June 15-21, 2009.

Summer School, Bratislava, Slovak Republic, June 15 – 21, 2009.

Co-author on Lecture on: Surface Electrochemistry of Metal Chalcogenides and their Bio-Organic Derivatives.



Wintersnow

D. Bedeaux

Workshop "Seventieth Birthday Professor Ola Hunderi", NTNU, Trondheim, March 27, 2009.

Lecture on: Optical Properties of Surfaces.

Visit Universite Libre de Bruxelles, Belgium, March 29 – April 1, 2009.

Guest Lecture on: Non-equilibrium Thermodynamics and Local Equilibrium for Surfaces.

Conference Eurotherm, Namur, Belgium, May 24 – 28, 2009.

Lecture on: Non-equilibrium Thermodynamics and Local Equilibrium for Surfaces.

17th Symposium on Thermophysical Properties, Boulder, Colorado, USA, June 21 – 26, 2009.

Organizer of the Session on Non-Equilibrium Thermodynamics.

Co-author on Lectures on: "Transport Coefficients of N-butane into and through the Surface of Silicalite-1 from Non-Equilibrium Molecular Dynamics Study" and "Transport Equations and Coefficients for Active Transport of Ca²⁺ ATPase Isoforms".

Conference IWNET2009, Cuernavaca, Mexico, Aug. 23 – 28, 2009. Lecture on: Non-equilibrium Thermodynamics and Local Equilibrium for the Liquid-Vapor Interface.

International Workshop on Non-Equilibrium Thermodynamics on the Occasion of Professor Signe Kjelstrup's 60th Birthday, Trondheim, Norway, Sep. 3 - 4, 2009.

Co-author on Lectures on: "Non-equilibrium Studies of "Hot" Water: from Bulk to Interfaces", "Non-equilibrium Thermodynamics of Interfaces with the Classical Density Functional Theory", "Diffusion of Butane, Heat Conduction and Thermal Diffusion into and through a Zeolite Membrane; a Study Using Non-Equilibrium Molecular Dynamics" and "Verification of Onsager's Reciprocal Relations for Evaporation and Condensation Using Non-Equilibrium Molecular Dynamics".

T. Berg

22nd Task Force Meeting of the ICP Vegetation, Braunschweig, Germany, Feb. 2 – 5, 2009.

Co-author on Lecture on: Strong and Weak Points of the Moss Biomonitoring Technique for Metal Deposition Studies – as illustrated from 30 Years of Experience in Norway.

Forest Mercury Meeting, Hafjell, Norway, March 18 – 20, 2009.

Co-Author on Lecture on: Reemission Measurements – Results so Far.

Field Work, Ny-Ålesund, Spitzbergen, April 20 – May 4 and August 17 - 31, 2009.

Conference PRiMO, Bourdeaux, France, May 17 – 19, 2009.

Co-author on Poster Presentation: Comparative Study on Acute Toxicity and Stress Gene Expression in *Calanus Finmarchicus* and *C. Glacialis* Following Mercury Exposure.

9th ICMGP, Guyang, China, June 7 – 12, 2009.

Co-Author on Lectures on: "Long-Term Antarctic Measurements of Atmospheric Mercury", "GEM Measurements During 8 Years at Zeppelin, Ny-Ålesund and its Relation to Climate", "Mercury (Hg) Speciation Measurements at the Zeppelin Air Monitoring Station, Ny-Ålesund, Svalbard", "Determination of Methyl Mercury in Arctic Aquatic Systems", "Mercury Exchange Between Air and Snow in Ny-Ålesund, Svalbard", "Comparative Study on Acute Toxicity and Stress Gene Expression in *Calanus Finmarchicus* and *C. Glacialis* Following Mercury Exposure" and "Seasonal Variation of Total Mercury (Hg), Metallothionein and Catalase in Black-Legged Kittiwake (*Rissa Tridactyla*)".

Co-author on Poster Presentations: "Bayelva: a high Arctic Proglacial Stream in Ny-Ålesund, Svalbard" and "Seasonal Changes in Mercury Accumulation in Zooplankton from an Arctic Marine Food Web".

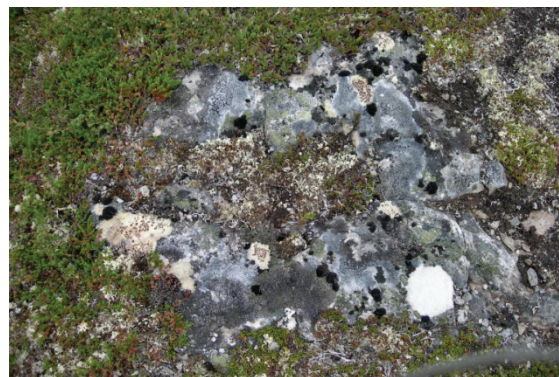
AMAP Meeting, Ottawa, Canada, Sept. 21 – Oct. 1, 2009.

M. Bjørgen

Research Stay at University of Oslo, Department of Chemistry, July 21 – 30, 2009.

T. Bruvoll

International Workshop on Non-Equilibrium Thermodynamics on the Occasion of Professor Signe Kjelstrup's 60th Birthday, Trondheim, Norway, Sep. 3 - 4, 2009.



Lichen on the rocks

O. Burheim

MOLTEN 2009, 8th International Conference on Molten Slags, Fluxes and Salts, Santiago, Chile, Jan. 18 – 21, 2009.

Co-author on Lecture on: Electrodeoxidation of Solid Fe₂O₃ in Molten CaCl₂ to Produce Iron.

Conference "Diagnostic Tools for Fuel Cells 2009", SINTEF Materialer og Kjemi, NTNU, Trondheim, June 23 – 24, 2009.

Co-author on Poster Presentation: Calorimetric Study of the PEMFC.

Fuel Cell Seminar 2009, Palm Springs, CA, USA, Nov. 16 – 19, 2009.

Co-author on Lecture on: A Calorimetric Analysis of a PEMFC and the Production of H₂O₂ at the Cathode.

Conference "Hydrogen and Fuel Cells in the Nordic Countries – 2009", Oslo, Norway, Nov. 24 – 26, 2009.

Co-author on Lecture on: A Calorimetric Analysis of a PEMFC and the Production of H₂O₂ at the Cathode.

P. Carlsen

Leave of Absence, Feb. 1 – Dec. 31, 2009.

C. Chu

SETAC Europe 19th Annual Meeting, Gothenburg, Sweden, May 31 – June 4, 2009.

Co-author on Poster Presentation: Model for Prediction of Marine Ecotoxicity of Solvents used for CO₂-Capture.

Activities

Co-author on Lecture on: Validation of Molecular Structures Sampled by Evolutionary Algorithms Using an Intuitive Screening Model.



From the rosegarden

P. – O. Eggen

Kjemiløypa 2009, NTNU, Trondheim, Feb. 24 – March 27, 2009.

Co-author on Lecture on: Kjemiløypa 2009.

"En eksperimentell skoledag". Interview in "Universitetsavisa", March 10, 2009.

Symposium "Learning by Doing: Experiments and Instruments in the History of Science Teaching", Regensburg, Germany, April 4 - 5, 2009.

Co-author on Lecture on: Icons from Electrochemistry and their Reconstruction in Teaching.

A. Fiksdahl

Section Leader, Organic Chemistry Group, Department of Chemistry, NTNU, Jan. 1 – Aug. 31, 2009.

Member of National Committee for 18th 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.

Conference "24. Organisk kjemisk vintermøte", Skeikampen, Norway, Jan. 8 - 11, 2009.

Co-author on Lecture on: "Cyclopenta[g]isoquinolin-5-ol from Pyridylmalonate" and "New Gold Catalysed Cyclisation of Diynes".

Co-author on Poster Presentation: Preparation of new Chiral NHC Ligands.

Conference "XVIII EuCheMS", Gothenburg, Sweden, June 22 – 25, 2009.

Co-author on Poster Presentation: New Gold Catalysed Cyclisation Reactions of 1,6-Diynes.

Conference 16th European Symposium on Organic Chemistry, Prague, Czech Republic, July 12 – 16, 2009.

Co-author on Poster Presentation: New Gold Catalysed Reaction of 1,6-Diynes.

15th International IUPAC Conference, Glasgow, UK, July 26 – 30, 2009.

Co-author on Poster Presentations: "Application of new Chiral NHC Ligands" and "New Gold Catalysed Reaction of 1,6-Diynes".

T.P. Flaten

Deputy Head of the Department of Chemistry.

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

Board Member, Norwegian Chemical Society, Trondheim Branch.

Editor, Norsk Epidemiologi (Norwegian Journal of Epidemiology).

"Kobler fluor til psykose". Interview in "Dagens Medisin", Oct. 29, 2009.

E. Fuglseth

Conference "24. Organisk kjemisk vintermøte", Skeikampen, Norway, Jan. 8 – 11, 2009.

Co-author on Lecture on: Asymmetric Reduction of Para-Substituted α -Fluoroacetophenones.

Co-author on Poster Presentation: Synthesis of New Potential Tyrosine Kinase Inhibitors.

O.R. Gautun

Conference "24. Organisk kjemisk vintermøte", Skeikampen, Norway, Jan. 8 – 11, 2009.

Co-author on Poster Presentation: Preparation of New Ru-salen Complexes for the Catalytic Asymmetric Aziridination of Olefins.

Opponent at Doctoral Defence, University of Oslo, Norway, March 13, 2009.

10th Tetrahedron Symposium, Paris, France, June 23 – 26, 2009.

Co-author on Poster Presentation: Asymmetric Catalytic Aziridination of 1,2-Dihydronaphthalenes.

K.F. Gebremariam

Participation at Summer School, Aristotle University, Thessaloniki, Greece, July 18 – Aug. 3, 2009.

K.S. Glavatskiy

13th International Conference on Surface and Colloid Science (ICSCS), New York, USA, June 13 – 20, 2009.

S.V. Gonzalez

MS Course and Training, Swansea University, UK, Sept. 7 – 26, 2009.

K. Hagen

13th European Symposium on Gas Electron Diffraction, Blaubeuren, Germany, June 24 – 28, 2009.

Co-author on Poster Presentation: Methyl Chloroacetate - Structure and Conformation.

L. van der Ham

8th World Congress of Chemical Engineering, Montreal, Canada, Aug. 23 – 27, 2009.

Co-author on Lecture on: Bringing the Theoretical Gains of Minimum Entropy Production into Practice: The Case of a H₂SO₄ Decomposition Reactor.

22nd International Conference on Efficiency, Cost, Optimisation, Simulation and Environmental Impact of Energy Systems, Iguassu Falls, Brazil, Aug. 31 – Sept. 3, 2009.

Co-author on Lecture on: Two Performance Indicators for Characterization of the Entropy Production in a Process Unit.



Amanita muscaria (Fly amanita)

Ø. Hestad

Research Co-Operation with Professor Steven Boggs at University of Connecticut, USA, July 2 – 17, 2009.

B.H. Hoff

Conference "24. Organisk kjemisk vintermøte", Skeikampen, Norway, Jan. 8 – 11, 2009.

Co-author on Lecture on: Asymmetric Reduction of Para-Substituted α -Fluoroacetophenones.

Co-author on Poster Presentations: "Regioselective C-6 Hydrolysis of Methyl O-Benzoyl Pyranosides Catalysed by Candida Rugosa Lipase", "Synthesis of Lignin Model Compounds" and "Synthesis of New Potential Tyrosine Kinase Inhibitors".

I. Inzoli

Working in Dhahran, Kingdom of Saudi Arabia, on Signe Kjelstrup's "Storforsk" Project: "Molecular Dynamics Simulations of two Component Phase Transitions", Jan. 1 – Dec. 31, 2009.

17th Symposium on Thermophysical Properties, Boulder, Colorado, USA, June 21 – 26, 2009.

Co-author on Lecture on: Transport Coefficients of N-butane into and through the Surface of Silicalite-1 from Non-Equilibrium Molecular Dynamics Study.

International Workshop on Non-Equilibrium Thermodynamics on the Occasion of Professor Signe Kjelstrup's 60th Birthday, Trondheim, Norway, Sep. 3 - 4, 2009.

Co-author on Lecture on: "Diffusion of Butane, Heat Conduction and Thermal Diffusion into and through a Zeolite Membrane; a Study Using Non-Equilibrium Molecular Dynamics".

1st Trondheim Gas Technology Conference, Trondheim, Norway, Oct. 21 – 22, 2009.

Co-author on Lecture on: Membrane Transport of N-butane by a Temperature Gradient.

S. Kjelstrup

20th International Conference of Statistical Mechanics, Taxco, Mexico, Jan. 6 – 9, 2009. Invited Key Note Lecturer.

38th Winter Meeting on Statistical Physics, Taxco, Mexico, Jan. 6 – 9, 2009.

Lecture on: Nature-Inspired Energy Efficient Design.

Professor in Part Time Position at TU Delft, Netherlands, Jan. 11 – 30, May 26 – July 15 and Oct. 17 – Nov. 1, 2009.

"Genesis, evolusjon og skapelse". Interview on Hopechannel.no, Jan. 16, 2009.

Trondheim Polyteknisk Forening, Feb. 25, 2009.
Lecture on: Brenselceller – hvorfor det?

17th Symposium on Thermophysical Properties, Boulder, Colorado, USA, June 21 – 26, 2009.

Co-author on Lectures on: "Transport Coefficients of N-butane into and through the Surface of Silicalite-1 from Non-Equilibrium Molecular Dynamics Study" and

"Transport Equations and Coefficients for Active Transport of Ca²⁺ ATPase Isoforms".

Activities

Conference "Diagnostic Tools for Fuel Cells 2009", SINTEF Materialer og Kjemi, NTNU, Trondheim, June 23 – 24, 2009.

Co-author on Poster Presentation: Calorimetric Study of the PEMFC.

8th World Congress of Chemical Engineering, Montreal, Canada, Aug. 23 – 27, 2009.

Co-author on Lecture on: Bringing the Theoretical Gains of Minimum Entropy Production into Practice: The Case of a H₂SO₄ Decomposition Reactor.

22nd International Conference on Efficiency, Cost, Optimisation, Simulation and Environmental Impact of Energy Systems, Iguassu Falls, Brazil, Aug. 31 – Sept. 3, 2009.

Co-author on Lecture on: Two Performance Indicators for Characterization of the Entropy Production in a Process Unit.

International Workshop on Non-Equilibrium Thermodynamics on the Occasion of Professor Signe Kjelstrup's 60th Birthday, Trondheim, Norway, Sep. 3 - 4, 2009.

Co-author on Lectures on: "Non-equilibrium Studies of "Hot" Water: from Bulk to Interfaces", "Nature-Inspired Engineering of a Polymer Electrolyte Membrane Fuel Cell", "Diffusion of Butane, Heat Conduction and Thermal Diffusion into and through a Zeolite Membrane; a Study Using Non-Equilibrium Molecular Dynamics", "The State of Minimum Entropy Production in Optimally Controlled Systems", "Reindeer Noses, Fluid Mechanics and Non-Equilibrium Thermodynamics" and "Verification of Onsager's Reciprocal Relations for Evaporation and Condensation Using Non-Equilibrium Molecular Dynamics".

1st Trondheim Gas Technology Conference, Trondheim, Norway, Oct. 21 – 22, 2009.

Co-author on Lecture on: Membrane Transport of N-butane by a Temperature Gradient.

Fuel Cell Seminar 2009, Palm Springs, CA, USA, Nov. 16 – 19, 2009.

Co-author on Lecture on: A Calorimetric Analysis of a PEMFC and the Production of H₂O₂ at the Cathode.

Committee Meeting "FRINAT" at the Research Council of Norway, Oslo, Nov. 23 – 24, 2009.

Conference "Hydrogen and Fuel Cells in the Nordic Countries – 2009", Oslo, Norway, Nov. 24 – 26, 2009.

Co-author on Lecture on: A Calorimetric Analysis of a PEMFC and the Production of H₂O₂ at the Cathode.

H. Koch

Research Stay at Universidad de Valencia, Spain, Jan. 3 – 7, Feb. 21 – March 1 and June 25 – July 11, 2009.

T. Kumelj

Bioinformatics Forum for Young Scientists (BFYS), Trondheim/Selbu, Norway, April 24 - 26 2009.

Co-author on Lecture on: Towards a Reactive Force Field for Fe (IV) with Application to Oxidative Dealkylation of DNA.



Thunderstorm approaching

S. Schnell Kvalvåg

1st Trondheim Gas Technology Conference, Trondheim, Norway, Oct. 21 – 22, 2009.

Co-author on Lecture on: Membrane Transport of N-butane by a Temperature Gradient.

L. Kvittingen

Kjemiløypa 2009, NTNU, Trondheim, Feb. 24 – March 27, 2009.

Co-author on Lecture on: Kjemiløypa 2009.

"Kjemiløype for 7. klassinger". Interview in the Journal "Tekna", 2/2009.

Symposium "Learning by Doing: Experiments and Instruments in the History of Science Teaching", Regensburg, Germany, April 4 - 5, 2009.

Co-author on Lecture on: Icons from Electrochemistry and their Reconstruction in Teaching.

A. Lervik

International Workshop on Non-Equilibrium Thermodynamics on the Occasion of Professor Signe Kjelstrup's 60th Birthday, Trondheim, Norway, Sep. 3 - 4, 2009.

Co-author on Lecture on: Non-equilibrium Studies of "Hot" Water: from Bulk to Interfaces.

S. Lierhagen

9th ICMGP, Guyang, China, June 7 – 12, 2009.

Co-author on Lecture on: Determination of Methyl Mercury in Arctic Aquatic Systems.

Co-author on Poster Presentation: Bayelva: a high Arctic Proglacial Stream in Ny-Ålesund, Svalbard.

8th International Sector Field ICPMS Conference, Gent, Belgium, Sep. 14 – 16, 2009.
Co-author on Poster Presentation: Mercury Speciation by RP HPLC/SF-ICP-MS with SC-2 FAST Autosampler.

T. Ljones

Conference "Biotrans 2009", Bern, Switzerland, July 5 – 10, 2009.
Co-author on Poster Presentation: Lipase Selectivity in Resolutions and Asymmetrisations. Allosteric effects.

A. Lykknes

Research Stay at Tokyo Institute of Technology, Japan, Jan. 1 - 13, 2009.
History of Science Seminar, Jan. 9, 2009.
Guest Lecture: Ellen Gleditsch: Professor, Radiochemist, and Mentor.

Kjemiløypa 2009, NTNU, Trondheim, Feb. 24 – March 27, 2009.
Co-author on Lecture on: Kjemiløypa 2009.

"Sjuendeklassinger lærer kjemi på NTNU". Interview in the Newspaper "Trønderbladet", March 17, 2009.

"En eksperimentell skoledag". Interview in "Universitetsavisa", March 10, 2009.

"Moro i kjemiløypa". Interview in the Newspaper "Sør-Trøndelag", March 25, 2009.

"Kjemiløype for 7. klassinger". Interview in the Journal "Tekna" 2/2009.

Research Stay in Braunschweig and Berlin, Germany. Visits to Archives of the Max Planck Society Berlin, Archives of the Physikalisch-Technische Bundesanstalt (PTB) Braunschweig and Berlin, Humboldt University Archives Berlin, Landesarchiv Berlin, Historical Archives of the Deutsches Technikmuseum Berlin, Geheimes Staatsarchiv Preussischer Kulturbesitz Berlin, April 19 – 30, 2009.

Workshop im Rahmen des FWF-Projektes "Geschichte der Österreichischen Kern Forschung im 20. Jahrhundert", Vienna, Austria, June 4 – 6, 2009.

Lecture on: The Norwegian-Austrian Connection: Ellen Gleditsch and her International Networks.

XXIII International Congress of History of Science and Technology: "Ideas and Instruments in Social Context", Budapest, Hungary, July 28 – Aug. 2, 2009.

Co-author on Lecture on: Ida and Walter Noddack: A Collaborating Couple in Chemistry. Co-organizer of symposium: "For Better or for Worse? Collaborative Couples in the Sciences".

7th International Conference on the History of Chemistry: "Consumers and Experts: the Uses of Chemistry (and Alchemy)", Sopron, Hungary, Aug. 2 – 5, 2009.

Lecture on: The Reception of the Periodic Table among Norwegian Chemists, c. 1870-1930s.

ESERA Conference 2009 (European Science Education Research Association), Istanbul, Turkey, Aug. 30 – Sep. 5, 2009.

Co-author on Lecture on: What Brought them into Science? University Students' Interest Profiles and Motivation for Choosing Science on University Level.

"Jubileumstreff kull '59 Kjemi NTH", Trondheim, Oct. 9, 2009.

Lecture on: "Hurra for 100-åringen! Noen glimt fra NTNUs og kjemiutdanningen i Trondheims historie, 1910-2010".

Meeting "MONS: Møte om norsk språk", NTNU, Trondheim, Nov. 26 – 28, 2009.

Co-author on Lecture on: "Å skrive informativ og utgreiende artikkel i naturfag på ungdomstrinnet og videregående skole: Hva er hensikten?".

M. Martinsen

Research Stay at Vancouver Island University, Department of Chemistry, Canada, July 8 – Aug. 16, 2009.

K. Mathisen

Research Stay at the European Synchrotron Radiation Facility (ESRF), Swiss-Norwegian Beam Line, Grenoble, France, Feb. 24 – March 3, April 14 – 28 and Oct. 22 – 27, 2009.

Synchrotron User Meeting, Lillehammer, Norway, June 17 – 19, 2009.

S. Melnes

Conference "24. Organisk kjemisk vintermøte", Skeikampen, Norway, Jan. 8 – 11, 2009.

Co-author on Poster Presentation: Preparation of New Ru-salen Complexes for the Catalytic Asymmetric Aziridination of Olefins.

10th Tetrahedron Symposium, Paris, France, June 23 – 26, 2009.

Co-author on Poster Presentation: Asymmetric Catalytic Aziridination of 1,2-Dihydronaphtalenes.

Activities

Ø. Mikkelsen

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

12th International Conference on Chemistry and the Environment ICCE 2009, Stockholm, Sweden, June 14 – 17, 2009.

Co-author on Lecture on: ATMS (Automatic Trace Metal System) for Early Warning and Short Term Event in Polluted Rivers.

“Schrödingers katt”. Interview NRK Vitenmagasin, Sep. 10, 2009.

Researcher's Night, NTNU, Trondheim, Sep. 25, 2009.

Lecture on: Miljøovervåking.

Åpen dag, UKA-09. Exhibition: "Vil du se hva noen av Norges skarpeste hjerner driver med?", NTNU, Trondheim, Oct. 11, 2009.

Lecture on: Miljøkjemikeren.

Research Stay for AURORA Mobility Project, NFR at Laboratoire PROTEE – équipe CAPTE, Université du Sud Toulon Var, La Garde, France, Nov. 18 – 27, 2009.

D.G. Nicholson

Head of the Department of Chemistry.

Chairman, SNX Council, Swiss-Norwegian Beamlines at the European Synchrotron Radiation Facility, Grenoble, France.

Scientific Advisory Council, Max IV Synchrotron Project, Max-Lab., Lund, Sweden.

Research stay at the European Synchrotron Radiation Facility (ESRF), Swiss-Norwegian Beam Line (SNBL), Grenoble, France, April 14 – 19 and Nov. 30 – Dec. 4, 2009.

SNX Council Meeting (SNBL), Lugano, Switzerland, June 5 – 13, 2009.

Planning MS-laboratory, University of Perugia, Italy, Sep. 23 – 28, 2009.



The old monastery in September

V. Partali

Section Leader, Organic Chemistry Group, Department of Chemistry, NTNU, Sep. 1 – Dec. 31, 2009.

Conference “24. Organisk kjemisk vintermøte”, Skeikampen, Norway, Jan. 8 – 11, 2009.

Co-author on Lectures on: “Carotenoids out of the Ordinary” and “Cationic Carotenoid Amphiphiles as Gene Transfection Vectors”.

Co-author on Poster Presentations: “Synthesis of Precursor Compounds for Carotenoid Cationic Lipids” and “The Secret Properties of DMF and DMSO”.

12th Annual Meeting American Society of Gene Therapy, San Diego, USA, May 27 – 30, 2009.

Co-author on Poster Presentation: A Novel Class of Rigid, Cationic Nucleic Acid Transfection Reagents Based on Carotenoid Lipids.

Workshop “Biophysics and Bioelectrochemistry of Biomimetic Structures”, Comenius University, Bratislava, Slovak Republic, June 15 – 21, 2009.

Co-author on Lectures on: “Carotenoid Aggregates of Predifined Size” and “Optical Resolution by Fractional Aggregation”.

“Kjemper mot aldring og kreft”. Interview in the Newspaper “Adresseavisen”, Sep. 24, 2009.

Research Co-Operation with Professor Maria Tsimidou, Aristotle University, Thessaloniki, Greece, Oct. 12 – 16 and Dec. 19 – 31, 2009.

T. Rolfsen

Planning MS-laboratory, University of Perugia, Italy, Sept. 23 – 28, 2009.

E. – M. Sandru

Conference “24. Organisk kjemisk vintermøte”, Skeikampen, Norway, Jan. 8 – 11, 2009.

Co-author on Lecture on: Carotenoids out of the Ordinary.

Participation on Summer School, Comenius University, Bratislava, Slovak Republic, June 15 – 21, 2009.

Co-author on Lecture on: Carotenoid Aggregates of Predifined Size.

R. Schmid

13th Norwegian Seminar on Mass Spectrometry, Hafjell, Øyer, Norway, Jan. 25 – 28, 2009.

8th International Sector Field ICPMS Conference, Gent, Belgium, Sep. 14 – 16, 2009.

Co-author on Poster Presentation: Mercury Speciation by RP HPLC/SF-ICP-MS with SC-2 FAST Autosampler.

1st Conference on Chemical Engineering and Advanced Materials (CEAM), Naples, Italy, Nov. 23 – Dec. 8, 2009.

Co-author on Lecture on: Influence of Fuel Oxygen on Diesel Combustion, Engine Performance, Ultrafine Particles, THC, CO, Smoke and NOx Emissions.

N. Simic

Field Work, Niš, Serbia, June 29 - July 3, 2009.

C. Sperger

Conference “24. Organisk kjemisk vintermøte”, Skeikampen, Norway, Jan. 8 – 11, 2009.

Co-author on Lecture on: New Gold Catalysed Cyclisation of Diynes.

Co-author on Poster Presentation: Preparation of New Chiral NHC Ligands.

Conference “XVIII EuCheMS”, Gothenburg, Sweden, June 22 – 25, 2009.

Co-author on Poster Presentation: New Gold Catalysed Cyclisation Reactions of 1,6-Diynes.

Conference 16th European Symposium on Organic Chemistry, Prague, Czech Republic, July 12 – 16, 2009.

Co-author on Poster Presentation: New Gold Catalysed Reaction of 1,6-Diynes.

15th International IUPAC Conference, Glasgow, UK, July 26 – 30, 2009.

Co-author on Poster Presentations: “Application of new Chiral NHC Ligands” and “New Gold Catalysed Reaction of 1,6-Diynes”.

A.O. Steen

Field Work, Ny-Ålesund, Spitzbergen, March 4 – 13, 2009.

9th ICMGP, Guyang, China, June 7 – 12, 2009.

Co-Author on Lectures on: “Mercury (Hg) Speciation Measurements at the Zeppelin Air Monitoring Station, Ny-Ålesund, Svalbard”, “Determination of Methyl Mercury in Arctic Aquatic Systems” and “Mercury Exchange Between Air and Snow in Ny-Ålesund, Svalbard”.

Co-author on Poster Presentation: Bayelva: a high Arctic Proglacial Stream in Ny-Ålesund, Svalbard.

E. Steinnes

Awarded the Guldberg-Waage-medal at the Norsk Kjemisk Selskaps Board Meeting, April 24, 2009.

22nd Task Force Meeting of the ICP Vegetation, Braunschweig, Germany, Feb. 2 – 5, 2009.

Lecture on: Strong and Weak Points of the Moss Biomonitoring Technique for Metal Deposition Studies – as illustrated from 30 Years of Experience in Norway.

33rd International Symposium on Remote Sensing, Stresa, Italy, May 4 – 8, 2009.

Lecture on: Soil and Health: Input from Soil Science to Human Health and Well-Being.

OECD Sustaining Soil Productivity in Response to Global Change, Madison, Wisconsin, June 29 – July 1, 2009.

Lecture on: Soil Quality and Human Health.

Seminar “Nuclear Physics Methods and Accelerators in Biology and Medicine”, Bratislava, Slovak Republic, July 5 – 15, 2009.

Lecture on: Radioecology.

5th International Workshop on Biomonitoring of Atmospheric Pollution, Buenos Aires, Argentina, Sep. 20 – 24, 2009.

Introductory Lecture on: Biomonitoring of Air Pollutants on the Local and Regional Scales Using Mosses: Strong and Weak Points.

V. Stockmann

Conference “24. Organisk kjemisk vintermøte”, Skeikampen, Norway, Jan. 8 - 11, 2009.

Co-author on Lecture on: Cyclopenta[g]isoquinolin-5-ol from Pyridylmalonate

15th International IUPAC Conference, Glasgow, UK, July 26 – 30, 2009.

Co-author on Poster Presentation: Application of new Chiral NHC Ligands.



Autumn in Trondheim

C.L. Øpstad

Conference “24. Organisk kjemisk vintermøte”, Skeikampen, Norway, Jan. 8 – 11, 2009.

Co-author on Lectures on: “Carotenoids out of the Ordinary” and “Cationic Carotenoid Amphiphiles as Gene Transfection Vectors”.

Co-author on Poster Presentations: “Synthesis of Precursor Compounds for Carotenoid Cationic Lipids” and “The Secret Properties of DMF and DMSO”.

Research Stay at Weill Cornell Medical College in Qatar, Doha, Qatar, May 19 – June 15, 2009.

Activities



The little lighthouse

12th Annual Meeting American Society of Gene Therapy, San Diego, USA, May 27 – 30, 2009.

Co-author on Poster Presentation: A Novel Class of Rigid, Cationic Nucleic Acid Transfection Reagents Based on Carotenoid Lipids.

Participating in 59th Meeting of Nobel Laureates (dedicated to Chemistry), Lindau, Germany, June 27 – July 4, 2009.

117th BASF International Summer Course, Ludwigshafen, Germany, July 21 – 31, 2009.

P. – O. Åstrand

Section Leader, Physical Chemistry Group, Department of Chemistry, NTNU, Jan. 1 - Aug. 31, 2009.

Leave of Absence, Sep. 1 – Dec. 31, 2009.

Bioinformatics Forum for Young Scientists (BFYS), Trondheim/Selbu, Norway, April 24 - 26 2009.

Co-author on Lecture on: Towards a Reactive Force Field for Fe (IV) with Application to Oxidative Dealkylation of DNA.

Visit at University of Copenhagen, Denmark, Sep. 3, 2009.

Guest Lecture on: Molecular Mechanics Models for Electronic Polarization.

Theory Group Meeting, Northwestern University, Evanston, Illinois, USA, Sep. 21, 2009.

Guest Lecture on: Molecular Mechanics Model for the Frequency-Dependent Polarizability.

Workshop "Multiscale Modeling and Simulation in Science", Stockholm, Sweden, Nov. 2 – 29, 2009.

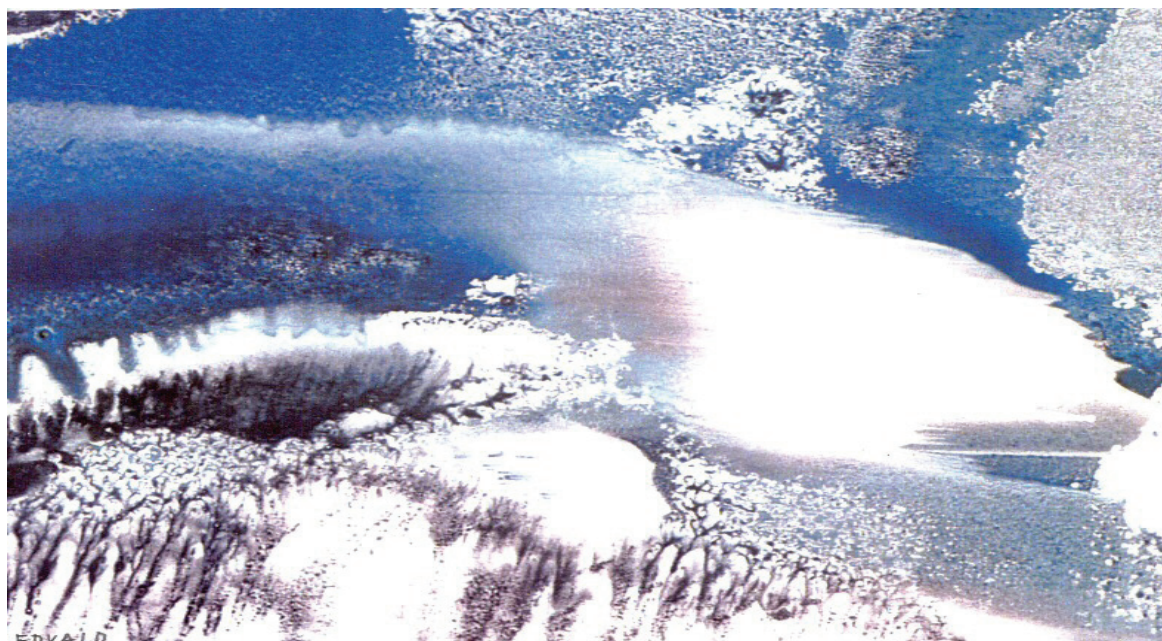
Lecture on: Electronegativity Equalization and Point Dipole Interaction Models: On the Scaling with the Size of the System.



The rivermouth of Nidelva in february

Spring examination

Course no.	Course title (credits)	Lectures and exercise coordinators	Candidates/Passed
RFEL1001	Natural Science and World Views (7,5)	Reidar Edvald Stølevik Karl Erik Zachariassen	52/47
KJ1020	Organic Chemistry (15)	Vassilia Partali	136/107
KJ2022	Spectroscopic Methods in Organic Chemistry (7,5)	Nebojsa Simic	29/21
KJ2043	Physical Methods in Structural Chemistry (15)	Morten Bjørgen	4/4
KJ2051	Analytical Chemistry, Advanced Course (7,5)	Øyvind Mikkelsen Florinel Gabriel Banica	15/14
KJ2053	Chromatography (7,5)	Anne Fiksdahl Rudolf Schmid	45/44
KJ2070	Environmental Chemistry (15)	Torunn Berg Trond Peder Flaten	32/28
KJ3055	Analytical Atomic Spectrometry (7,5)	Florinel Gabriel Banica	7/7
KJ3065	Enzyme chemistry (7,5)	Torbjørn Ljones	1/1
KJ8100	Organic Medicinal and Pharamaceutical Chemistry (7,5)	Derek James Chadwick	17/15
KJ8106	Advanced Organic Chemistry (7,5)	Per Henning Carlsen	-
KJ8200	Spectroscopy and Chemometrics (7,5)	Bjørn Kåre Alsberg	1/1
KJ8204	Quantitative Structure-Activity Relationships (7,5)	Bjørn Kåre Alsberg	-
KJ8205	Molecular Modelling (7,5)	Per-Olof Åstrand	-
KJ8208	Advanced Irreversible Thermodynamics (6)	Signe Kjelstrup	2/2
KJ8901	Enzyme chemistry (7,5)	Torbjørn Ljones	-
TKJ4111	Organic Chemistry, Advanced Course (7,5)	Bård Helge Hoff	16/13
TKJ4130	Organic Synthesis, Laboratory (7,5)	Bård Helge Hoff Vassilia Partali	10/10
TKJ4135	Organic Synthesis, Advanced Course (7,5)	Odd Reidar Gautun	10/9
TKJ4160	Basic Physical Chemistry and Laboratory (15)	Signe Kjelstrup Henrik Koch	79/57
TKJ4166	Chemical Bond Theory and Spectroscopy (7,5)	Henrik Koch	23/16
TKJ4175	Chemometrics, Basic Course (7,5)	Bjørn Kåre Alsberg	3/3
TKJ4190	Physical Chemistry, Project Work (7,5)	Morten Bjørgen	1/1



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Graduate Students

Autumn examination

Course no.	Course title (credits)	Lectures and exercise coordinators	Candidates/Passed
KJ1000	General Chemistry (15)	Kolbjørn Hagen Torbjørn Ljones	213/191
KJ1030	Inorganic Chemistry (15)	Tor Grande Mari-Ann Einarsrud	43/38
KJ1040	Physical Chemistry (15)	Morten Bjørgen Astrid Lund Ramstad Florinel Gabriel Banica	29/24
KJ2031	Inorganic Chemistry, Advanced Course (7,5)	Karina Mathisen	14/14
KJ2050	Analytical Chemistry, Basic Course (7,5)	Øyvind Mikkelsen Florinel Gabriel Banica	29/27
KJ2090	Chemistry Education - Chemistry Dissemination (7,5)	Vivi Ringnes	7/7
KJ2091	Teacher training/dissemination project in chemistry (7,5)	Lise Kvittingen	-
KJ3001	Stereochemistry and Synthesis of Chiral Compounds (7,5)	Per Henning Carlsen	-
KJ3005	Organometallic Compounds in Organic Synthesis (7,5)	Odd Reidar Gautun	11/11
KJ3021	Nuclear Magnetic Resonance Spectroscopy (7,5)	Nebojsa Simic	19/15
KJ3050	Marine Organic Environmental Chemistry (7,5)	Øyvind Mikkelsen	19/19
KJ3053	Analytical Methods for Industrial- and Environmental Monitoring (7,5)	Øyvind Mikkelsen	3/3
KJ3056	Chemical and Sensors and Biosensors (7,5)	Florinel Gabriel Banica	2/2
KJ3058	Analytical Chemical Separation Techniques (7,5)	Rudolf Schmid	1/1
KJ3070	Advanced Aquatic Chemistry (15)	Trond Peder Flaten	26/26
KJ3071	Applied geochemistry (7,5)	Rolf Tore Ottesen	15/15
RFEL3093	Episodes from the history of science (7,5)	Annette Lykknes	9/9
RFEL8093	Episodes from the history of science (10)	Annette Lykknes	-
KJ6002	Basic Chemistry 2 (Continuing education for teachers) (7,5)	Lise Kvittingen	13/13
KJ8021	Stereochemistry and Synthesis of Chiral Compounds (7,5)	Per Henning Carlsen	-
KJ8053	Analytical Methods for Industrial- and Environmental Monitoring (7,5)	Øyvind Mikkelsen	1/1
KJ8056	Chemical and Sensors and Biosensors (7,5)	Florinel Gabriel Banica	1/0
KJ8070	Advanced Aquatic Chemistry (15)	Trond Peder Flaten	5/5
KJ8104	New Methods in Organic Synthesis (7,5)	Anne Fiksdahl	-
KJ8105	Organometallic Compounds in Organic Synthesis (7,5)	Odd Reidar Gautun	3/3
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
KJ8902	Computational Chemistry (7,5)	Per-Erik Larsson	3/3
TKJ4100	Basic Organic Chemistry and Laboratory (15)	Odd Reidar Gautun	89/66
TKJ4170	Quantum Chemistry, Advanced Course (7,5)	Henrik Koch	-
TKJ4180	Physical Organic Chemistry (7,5)	Rudolf Schmid	12/6
TKJ4195	Chemometrics, Advanced Course (7,5)	Bjørn Kåre Alsberg	1/1
TKJ4200	Irreversible Thermodynamics (7,5)	Signe Kjelstrup	8/6
TKJ4205	Computational Chemistry (7,5)	Per-Erik Larsson	7/7
TKJ4215	Statistical Thermodynamics in Chemistry and Biology (7,5)	Øystein Hestad	22/22
TKJ4510	Physical Chemistry, Specialization Project (15)	Morten Bjørgen	3/3
TKJ4515	Physical Chemistry, Specialization Course (7,5)	Morten Bjørgen	2/2
TKJ4520	Organic Chemistry, Specialization Project (15)	Odd Reidar Gautun	5/5
TKJ4525	Organic Chemistry, Specialization Course (7,5)	Anne Fiksdahl	2/2

Re-sit examination

Course no.	Course title (credits)	Lectures and exercise coordinators	Candidates/Passed
RFEL1001	Natural Science and World Views (7,5)		44/39
KJ1000	General Chemistry (15)		18/6
KJ1020	Organic Chemistry (15)		8/6
KJ1030	Inorganic Chemistry (15)		2/2
KJ1040	Physical Chemistry (15)		4/1
KJ2022	Spectroscopic Methods in Organic Chemistry (7,5)		5/3
KJ2050	Analytical Chemistry, Basic Course (7,5)		1/1
KJ2051	Analytical Chemistry, Advanced Course (7,5)		1/1
KJ2070	Environmental Chemistry (15)		4/2
KJ3021	Nuclear Magnetic Resonance Spectroscopy (7,5)		2/2
KJ3055	Analytical Atomic Spectrometry (7,5)		7/7
RFEL8093	Episodes from the history of science (10)		1/1
KJ8052	Analytical Electrochemistry and its Application within Industrial and Environmental Monitoring (7,5)		4/4
KJ8100	Organic Medicinal and Pharmaceutical Chemistry (7,5)		17/15
KJ8104	New Methods in Organic Synthesis (7,5)		1/1
KJ8204	Quantitative Structure-Activity Relationships (7,5)		1/1
TKJ4100	Basic Organic Chemistry and Laboratory (15)		10/6
TKJ4111	Organic Chemistry, Advanced Course (7,5)		1/1
TKJ4160	Basic Physical Chemistry and Laboratory (15)		18/4
TKJ4180	Physical Organic Chemistry (7,5)		1/1



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Post Graduate Students

Siv.ing. students

3. year (MTKJ)

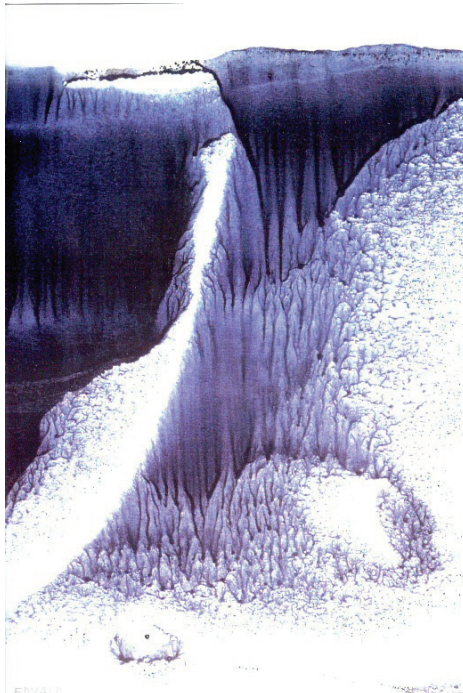
Bergersen, Amund Dolva
Ellila, Georg
Elnan, Jørund
Gulbrandsen, Tore Aarhus
Han, Jin
Isaksen, Stian Moe
Kaur, Maya
Larsen, Synne
Myhre, Rolf Heilemann
Solemslie, Henrik Winther
Strand, Mikael
Surdal, Cecilie
Tveekrem, Marit Elise Endresen
Vo, Mong Truc

4. year (MTKJ)

Austdal, Marie
Blakstad, Guro
Bugge, Steffen
Bøe, Maren Seljenes
Kaasa, Kristin
Nerem, Elisabeth
Solvang, Tina
Tungen, Jørn Eivind

5. year (MTKJ)

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



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Master students in progress

Chemistry (MKJ)

Berge, May Britt
Borkenhagen, Marius
Braaten, Hans Fredrik Veiteberg
Edvardsen, Tove-Nanny
Egede-Nissen, Cecilie
Engøy, Ingemund Magnus Falkberget
Haug, Siri
Heggøy, Anette
Helgerud, Trygve
Hjertenæs, Eirik
Hoftaniska, Idar
Hovde, Gunnhild
Høyvik, Ida-Marie
Martinsen, Morten
Nauste, Kristian Bunkholt
Ohm, Ragnhild Gaard
Sivertsen, Sveinung Sundfør
Skorpa, Ragnhild
Sveinhaug, Krister
Volynkin, Andrey Sergeevich
Aaen, Ingrid

Environmental toxicology and chemistry (MFORU)

Granly, Toril

Environmental toxicology and chemistry (MSENVITOX)

Alston, John Fraser
Bechmann, Pernille
Eskeland, Maren
Høydal, Liv Mari Brunstad
Haakseth, Anne-Britt
Kamalia, Uswatun Hasanah Isna
Larsen, Katrine Hervik
Liu, Zhucheng
Melting, Kine
Slinde, Gøril Aasen
Sundeng, Kathrine Helen
Trefjord, Terese

Master of Science Education (MLREAL)

Belsaas, Kristin
Houston, Audhild
Milli, Guri Kristine

Natural Resource Management (MSNARM)

Som, Bozume

The following ph.d. projects are in progress:

Student	Title	Thesis advisor
Chu, Chunmei	Automated de novo 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 fluoreerte 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
Gerontas, Apostolos	A history of the development of column chromatography: From Tswet to HPLC	Annette Lykknes
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 høg elektrisk felt påkjenning.	Per-Olof Åstrand
Iftekhar, Shafia	Trace metals and natural organic matters in rivers.	Torunn Berg
Kaspersen, Svein Jacob	New pyrrolo, thieno and furopyrimidine targeting tyrosine kinases (cancer) and protozoas: synthesis and bioactivity	Bård Helge Hoff
Kristiansen, Tina	Aerogels: A new class of materials for catalytic purposes.	David G. Nicholson
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
Martinsen, Morten	Development of an on-line monitoring platform and procedure for rapid environmental and process monitoring of heavy oil extraction operations and industrial activity	Øyvind Mikkelsen
Melnes, Silje	Rational drug design synthesis of potential selective inhibitors of tyrosin kinase 2.	Odd Reidar Gautun
Mohsin, Muhammad Ali	Surface functionalization by bio-organic materials.	Florinel G. Banica

Post Graduate Students

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	Synthese av høy umettete bioorganiske forbindelser. (Synthesis of highly unsaturated bioorganic compounds.)	Vassilia Partali
Sæpurahman	Spectroscopic studies of zeolites and zeolite facilitated oxygenate/hydrocarbon conversion reactions	Morten Bjørgen
Smalø, Hans Sverre	Molecular models of electronic processes in Per-Olof Åstrand liquids.	
Steen, Anne Orderdalen	Atmosfærisk spesiering av kvikksølv i polare områder.	Torunn Berg
Stockmann, Vegar	Synthetic applications of nitropyridine derivatives.	Anne Fiksdahl
Strand, Ragnhild B.	Heterocyclic synthetic chemistry based on nitropyridine derivatives.	Anne Fiksdahl
Strasunske, 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
Thvedt, Thor Håkon Krane	Enzymatic resolution coupled with in-situ racemisation for production of enantiopure amines. Application of the building blocks in preparation of potential antifungal compounds.	Bård Helge Hoff
Zaidi, Asma	Highly unsaturated fatty acids as antennas for ligand enhanced lanthanide luminescence.	Vassilia Partali
Zeeshan, Muhammad	Optical resolution by fractional aggregation.	Vassilia Partali
Voldsund, Mari	Entropy production in process equipment	Signe Kjelstrup
Weggeberg, Hanne	Metal characterization of different size fractions of airborne particulate matter and adverse health effects in humans	Trond Peder Flaten
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

MSc in Chemistry 2009

Berge, Øystein Rønning	Hva karakteriserer byjord? Fordeling av arsen, utvalgte tungmetaller, PAHsum16 og PCBsum7 i tre norske byer
Supervisor:	Professor II Rolf Tore Ottesen
Examiners:	Chief Engineer, dr.scient. Bjørn Ove Berthelsen, Trondheim kommune Associate Professor Rudolf Schmid
Bøyesen, Katrine Lie	Characterization of Vanadium Species in Zeotypes for Redox Applications
Supervisors:	Professor David Nicholson Post.doc. Karina Mathisen
Examiners:	Research Scientist Bjørnar Arstad, SINTEF Associate Professor Morten Bjørgen
Delic, Asmira	Characterization of Copper Cations in Zeolite Y in Presence of Silver Cations; The Two-Cation Effect
Supervisors:	Professor David Nicholson Post.doc. Karina Mathisen
Examiners:	Research Scientist Bjørnar Arstad, SINTEF Associate Professor Hilde Lea Lein, Department of Materials Science and Engineering
Grave, Anlaug Haukvik	An in situ XAS study on the redox properties of chromium species in CrAPO-5 and the effect of cotemplating
Supervisors:	Professor David Nicholson Post.doc. Karina Mathisen
Examiners:	Research Scientist Merete Hellner Nilsen, UiO Associate Professor Morten Bjørgen
Holt, Yngvil	Jordforurensning i Porsgrunn. Kartlegging av tungmetaller og arsen i overflatejord i Porsgrunn kommune, Norge
Supervisor:	Professor II Rolf Tore Ottesen Associate Professor Trond Peder Flaten
Examiners:	Chief Engineer, dr.scient. Bjørn Ove Berthelsen, Trondheim kommune Associate Professor Rudolf Schmid
Hystad, Madeleine	The distribution and impact of chromium impurities in compensated SoG-silicon
Supervisors:	Associate professor Astrid Lund Ramstad Professor Lars Arnberg, Department of Materials Science and Engineering
Examiners:	Head of Research Tanja Pettersen, SINTEF Professor Otto Lohne, Department of Materials Science and Engineering
Jonassen, Hilding	Synthesis of highly unsaturated imines and amines
Supervisors:	Professor Vassilia Partali Dr.rer.nat. Richard Sliwka
Examiners:	Associate Professor Birte J. Sjursnes, HiØ Dr.techn., ph.d. Eva Henmo Mørkved
Kaspersen, Svein Jacob	Syntetiske transformasjoner av α -(3-pyridyl)malonat
Supervisor:	Professor Anne Fiksdahl
Examiners:	Professor Jan Skramstad, UiO Professor Emeritus Jan Magnus Bakke
Kristiansen, Tina	Growth Limitations of Copper Nanoparticles in Silica Aerogels: An In Situ XAS Study
Supervisors:	Professor David Nicholson Post.doc. Karina Mathisen
Examiners:	Research Scientist, dr.scient. Merete Hellner Nilsen, UiO Associate Professor Stian Svelle, UiO Professor Mari-Ann Einarsrud, Department of Materials Science and Engineer

Post Graduate Students

Lie, Aleksander Supervisors:	Asymmetrisation of prochiral 1,3-propanediols by enzyme-catalysed acetylation Associate professor Bård Helge Hoff Professor Torbjørn Ljones
Examiners:	Professor Emeritus Thorleif Anthonen Associate Professor Eirik Sundby, HiST Dr.techn. Helge Kjøsén
Næss, Mari Kirkebøen Supervisors:	Synthesis and Characterisation of Silver Substituted Aluminiumphosphates; Microporous Materials as Possible Carriers of Silver Nanoclusters Professor David Nicholson Post.doc. Karina Mathisen
Examiners:	Associate Professor Stian Svelle, UiO Associate Professor Hilde Lea Lein, Department of Materials Science and Engineering
Siegesmund, Øyvind Torbjørn Supervisor:	Development and electrochemical characterization of ultra-micro sensors using nanotechnology Professor Øyvind Mikkelsen Ph.d. Silje Marie Skogvold Professor Emeritus Knut Schrøder
Examiners:	Stipendiat Kristina Strasunske
Thvedt, Thor Håkon Krane Supervisor:	Syntese av α -fluorketoner, og rasemiske og enantiomert rene 2-fluoraminer Associate Professor Bård Helge Hoff
Examiners:	Research Scientist, dr.ing. Harald Svensen, Epax Dr. techn., ph.d. Eva Henmo Mørkved
Tynes, Mari Klevberg Supervisors:	In situ XAS Studies on the redox properties of titanium substituted zeotypes Professor David Nicholson Post.doc. Karina Mathisen
Examiners:	Research Scientist, dr.scient. Merete Hellner Nilsen, UiO Associate Professor Morten Bjørgen
Valvik, Beate Supervisors:	In-situ XAS Studies on Gold Species in Zeotypic Systems for the Oxidation of Carbon Monoxide Professor David Nicholson Post.doc. Karina Mathisen
Examiners:	Associate Professor Stian Svelle, UiO Associate Professor Morten Bjørgen

MSc in Chemistry/Siv.ing.

Berg, Michel Brunes Supervisors:	Polychlorinated biphenyls (PCBs) along an East - West transect Associate Professor Trond Peder Flaten Professor Emeritus Eiliv Steinnes
Examiners:	Senior Research Scientist, dr.scient. Per Johan Brandvik, SINTEF Associate Professor Trond Peder Flaten
Krakeli, Tor Arne Supervisor:	Asymmetrisk overføringshydrogenering av fluorholdige 1-naftylketoner Associate Professor Bård Helge Hoff
Examiners:	Cand.real. Reinert Fure Associate Professor Bård Helge Hoff
Kvalvåg, Sondre Schnell Supervisor:	A fluctation method to calculate partial molar quantities from molecular dynamics simulations Professor Signe Kjelstrup
Examiners:	Principal Engineer, dr.ing. Audun Røsjorde, Statoil Professor Signe Kjelstrup
Landsem, Eva Supervisor:	Synthesis studies towards potential therapeutic agents against multiple myeloma (blood cancer) Associate Professor Odd Reidar Gautun
Examiners:	Associate Professor Kåre Bredeli Jørgensen, UiS Associate Professor Odd Reidar Gautun

Mui, Vivian Wing Laam	Analysis of triethylene glycol (TEG), monoethylene glycol (MEG) and 2-methoxyethanol in natural gas using thermal desorption and two-dimensional gas chromatography
Supervisors:	Associate Professor Rudolf Schmid Head Engineer Torbjørn Vegard Løkken Dr.philos. Ståle Johnsen, Statoil
Examiners:	Associate Professor Rudolf Schmid
Ringholm, Magnus	Electronegativity Equalization in Molecular Mechanics
Supervisor:	Professor Per-Olof Åstrand
Examiners:	Professor Kenneth Ruud, UiT Professor Per-Olof Åstrand
Strand, Lilian Helene Sola	Gold catalyzed cyclization reactions of 1,6-diyne
Supervisor:	Professor Anne Fiksdahl
Examiners:	Professor Mats Tilset, UiO Professor Anne Fiksdahl
Sørensen, Benedicte Riise	Synthesis of Cationic Carotenoid Lipids Sensitive to Reduction
Supervisor:	Professor Vassilia Partali Stipendiat Christer L. Øpstad Associate Professor Michael D. Pungente, Weill Cornell Medical College in Qatar
Examiners:	Associate Professor Birte J. Sjørsnes, HiØ Professor Vassilia Partali
Sørum, Christopher	Synthesis of New Tyrosine Kinase Inhibitors
Supervisor:	Associate Professor Bård Helge Hoff
Examiners:	Associate Professor Kåre Bredeli Jørgensen, UiS Associate Professor Bård Helge Hoff
Voldsund, Mari	Modelling Distillation with Non-Equilibrium Thermodynamics
Supervisor:	Professor Signe Kjelstrup
Examiners:	Principal Engineer, dr.ing. Audun Røsjorde, Statoil Professor Signe Kjelstrup
Wilhelmsen, Øivind	The state of minimum entropy production in reactor design
Supervisors:	Professor Signe Kjelstrup Senior Project Engineer, dr.ing. Margrete Wesenberg, Statoil
Examiners:	Project Engineer, dr.ing. Eivind Johannessen, Statoil Professor Signe Kjelstrup
Åstrand, Ove Alexander	Synthesis of Novel Ruthenium-salen Complexes for the Asymmetric Aziridination of Olefins for the Preparation of Substituted 2—Aminotetralines
Supervisor:	Associate Professor Odd Reidar Gautun
Examiners:	Associate Professor Tore Lejon, UiT Associate Professor Odd Reidar Gautun

MSc in Education, chemistry

Dahl, Anette	Förändring över tid i koncentration av metaller i naturlig jord på Sørlandet i Norge
Supervisors:	Associate Professor Trond Peder Flaten Professor Emeritus Eiliv Steinnes
Examiners:	Chief Engineer, dr.scient. Bjørn Ove Berthelsen, Trondheim kommune Professor Torunn Berg
Sæth, Erlend Solveigson	Bruk av ICP-MS på filtrerte og ufiltrerte prøver og test av DGT for studier av metallers mobilitet i myr og våtmark med avrenning til vassdrag
Supervisor:	Professor Øyvind Mikkelsen
Examiners:	Professor Emeritus Knut Schrøder Professor Øyvind Mikkelsen

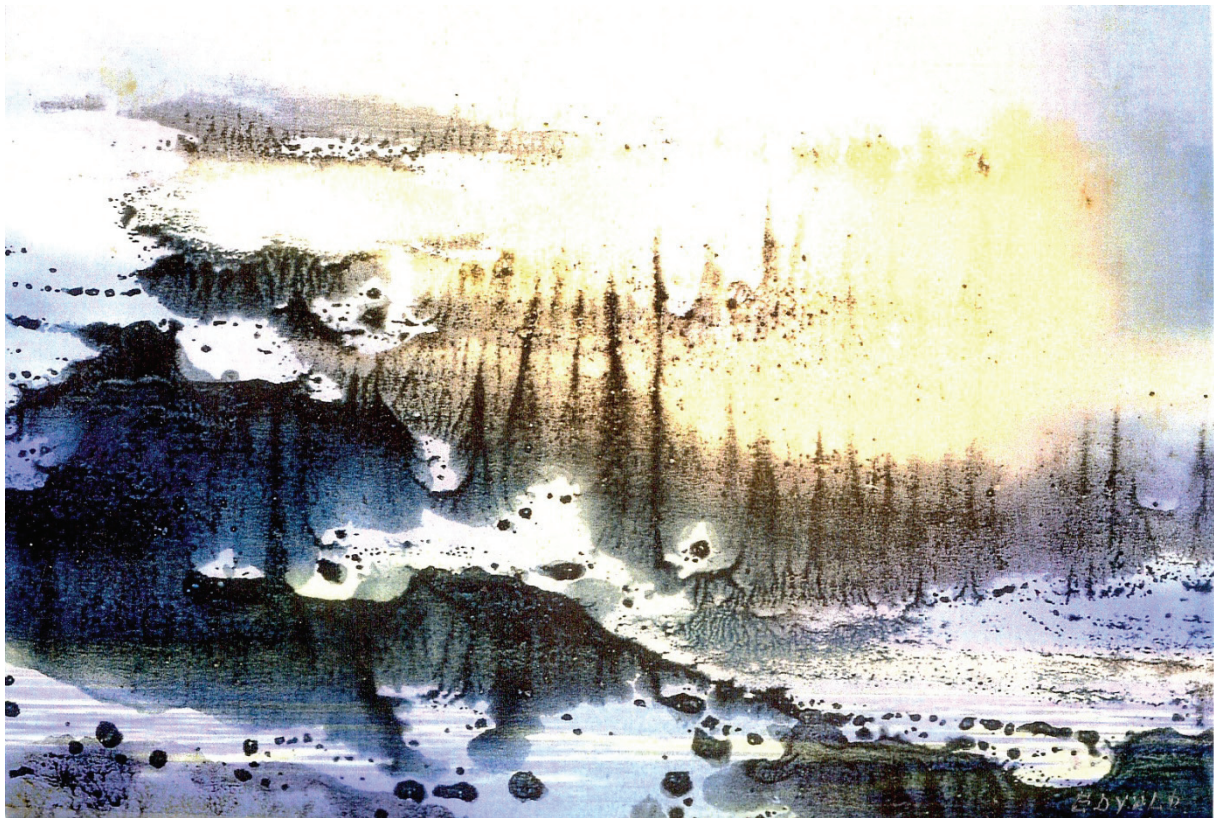
Post Graduate Students

MSc in Environmental toxicology and chemistry (MFORU)

Ottemo, Vivian Grønhaug
Supervisor: Sporelementer i gaupe i Norge
Associate Professor Trond Peder Flaten
Senior Research Scientist Hans Christian Pedersen, NINA
Professor Emeritus Eiliv Steinnes
Head Engineer Syverin Lierhagen
Examiners: Senior Research Scientist John Atle Kålås, NINA

Master project, exchange students

Paul, Jean-Nicolas
Supervisor: Use of solid electrodes in differential pulse anodic stripping voltammetry to detect various metals in water and nickel plating solutions
Professor Øyvind Mikkelsen
Examiners: Professor Emeritus Knut Schrøder
Ph.d. Silje Marie Skogvold



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Ph.d. in Chemistry

Andreassen, Trygve

Trial lecture
Supervisor
Evaluation committee

New methods for preparation of optically active unsaturated amines

Recent advances in synthesis of non-natural amino acids.
Associate Professor Odd Reidar Gautun
Professor Pher G. Andersson,
Department of Biochemistry and Organic Chemistry, Uppsala University
Professor Lise-Lotte Gundersen,
Department of Chemistry, University of Oslo, Norway
Professor Per Henning Carlsen,
Department of Chemistry, NTNU

Burheim, Odne Stokke

Trial lecture
Supervisor
Co-supervisor:

Evaluation committee

Thermal signatures and thermal conductivities of PEM fuel cells

Energy supply and sustainability for electric vehicles – Batteries vs. fuel cells.
Professor Signe Kjelstrup
Dr.ing. Preben J.S. Vie,
Institute for Energy Technology, Kjeller
Professor Ned Djilali,
Institute for Integrated Energy Systems, University of Victoria, Canada
Project Manager Dr.ing. Rune Halseid, Statoil ASA, Lillestrøm
Associate Professor Frode Seland, Department of Materials Science and Engineering, NTNU

Glavatskiy, Kirill Sergeevich

Trial lecture
Supervisor
Co-supervisors
Evaluation committee

Multicomponent evaporation and condensation as described by the square gradient model

The Jarzynski equation and the fluctuation theorem.
Professor Il Dick Bedeaux
Professor Signe Kjelstrup, Department of Chemistry, NTNU
Professor Joachim Gross, Technical University Delft, Engineering Thermodynamics, Delft, The Netherlands
Professor Gian Paolo Beretta, Università de Brescia, Brescia, Italy
Professor Tor Ytrehus, Department of Energy and Process Engineering, NTNU

Gonzalez, Susana Villa

Trial lecture
Supervisor
Evaluation committee

Optically active surfactants from the tartaric acids. Synthesis and properties

The origin of life: Chemical approaches.
Professor Per Henning Carlsen
Professor Gianfranco Savelli, Department of Chemistry, University of Perugia, Italy
Associate Professor Kåre Bredeli Jørgensen, Department of Mathematics and Natural Sciences, University of Stavanger
Professor Vassilia Partali, Department of Chemistry, NTNU

Haas, Ole-Erich

Trial lecture

Supervisor
Co-supervisor:
Evaluation committee

Transport on a nanoscale; quasi-elastic neutron scattering and molecular dynamics studies

Fuel cells – myths and facts (a sober discussion on the prospects and current limitations on the use of fuel cells).
Associate Professor Astrid Lund Ramstad
Professor Signe Kjelstrup, Department of Chemistry, NTNU
Professor Peter Pfeifer, Department of Physics and Astronomy, University of Missouri-Columbia, USA
Researcher Magnus Sørby, Institute for Energy Technology, Norway
Professor Henrik Koch, Department of Chemistry, NTNU

Post Graduate Students

Skogvold, Silje Marie

Trial lecture
Supervisor
Co-supervisor
Evaluation committee

Development and properties of nontoxic solid electrodes for environmental surveillance. Application in automatic on site determination of metals in natural water and industrial solutions

The importance of metal speciation.
Professor Øyvind Mikkelsen
Professor Emeritus Knut Henning Schrøder, Department of Chemistry, NTNU
Professor CMG van den Berg, Earth and Ocean Sciences, University of Liverpool, UK
Senior Scientist Ivanka Pizeta, Laboratory for Physical Chemistry of Traces, Centre for Marine and Environment Research, Ruder Boskovic Institute, Croatia
Professor Torunn Berg, Department of Chemistry, NTNU

Xu, Jing

Trial lecture

Supervisor
Co-supervisors
Evaluation committee

Transport phenomena in a temperature gradient studied by NEMD. A chemical reaction and phase transition

Computational approaches to model the phase behaviour of molecular liquids and solids: Water as an example. Discuss the state-of-the-art and the future potential of tools to model phase behaviour.
Professor Signe Kjelstrup
Professor Il Dick Bedeaux, Department of Chemistry, NTNU
Dr. Fernando Bresme, Department of Chemistry, Imperial College London, UK
Research Scientist Eirik Falck da Silva, Process Technology, SINTEF Materials and Chemistry, Trondheim
Professor Bjørn Kåre Alsberg, Department of Chemistry, NTNU



Collecting samples of seawater from the Trondheim fjord

Student Exchange from NTNU, Department of Chemistry

Name	Specialization	Level	Institution
Blakstad, Guro	MTKJ-Org.chem.	MSc, 4th yr	Háskóli Islands, Iceland
Bøe, Maren Seljenes	MTKJ-Org.chem.	MSc, 3th yr	University of California, Berkeley, USA
Egede-Nissen, Cecilie	MKJ-Analyt.chem.	MSc, 4th yr	Vrije Universiteit Brussel, Belgium
Heggøy, Anette	MKJ- Envir.chem.	MSc, 4th y	University of British Columbia, Canada
Høyvik, Ida-Marie	BKJ-Struct.chem.	BSc, 4th yr	Aarhus Universitet, Denmark
Lyngvi, Eirik	MTKJ-Org.chem.	MSc, 4th yr	University of California, Berkeley, USA
Mekki, Miriam	MTKJ-Phys.chem.	MSc, 5th yr	Universiteit Delft, Netherlands
Wilhelmsen, Øyvind Switzerland	MTKJ-Phys.chem.	MSc, 5th yr	Technische Hochschule Zürich,
Willassen, Veronica	MTKJ-Org.chem.	MSc, 4th yr	Technische Universität München, Germany

Student exchange to NTNU, Department of Chemistry

Name	Institution
Bock, Robert	Technische Universität, Berlin, Germany
Brycht, Mariola	University of Lodz, Poland
Chylík, Jan	Czech Yecgnical University, Prague, Czech Republic
Diedrich, Daniela	Georg-August-Universität Göttingen, Germany
Feige, Pascal	Fachhochschule Nordwestschweiz, Switzerland
Fuchs, Andreas	Philipps-Universiät Marburg, Germany
Koperek, Marta	University of Lodz, Poland
Lampert, Hannah	RWTH, Aachen, Germany
Lohse, Maria	TU Bergakademie Freiberg, Germany
Nick, Thomas	Georg-August-Universität Göttingen, Germany
Paul, Jean-Nicolas	Université des Sciences et Technologies, Lille, France
Petroix, Eve	ENSIACET, Toulouse, France
Primpke, Sebastian	Georg-August-Universität Göttingen, Germany
Rebmann, Edouard	University of Rouen, France
Schiefer, Frank	RWTH, Aachen, Germany
Superville, Pierre-Jean	USTL, Lille, France
Voss, Georg	RWTH, Aachen, Germany
Zilch, Rebecca	Georg-August-Universität Göttingen, Germany



A gray February morning at the pier

Staff

Academic Staff

Organic Chemistry



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



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



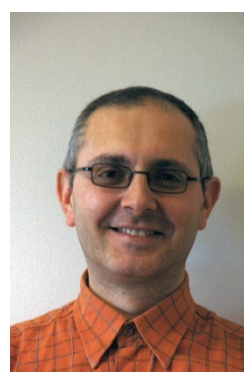
Professor, Dr.ing.
Anne Fiksdahl



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
Professor, Dr.scient.
Bjørn Alsberg



Assistant Professor
Terje Bruvoll



Professor, Ph.D. (Madison)
Torbjørn Ljones



Associate Professor, Dr.scient.
Astrid Lund Ramstad



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

Staff

Environmental and Analytical Chemistry



Group Leader
Dr.Scient
Øyvind Mikkelsen



Professor, Dr.scient.
Lise Kvittingen



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



Associate Professor, Dr.ing.
Florinel G. Banica



Ph.D.
Karina Mathisen



Associate Professor, Phd,
Annette Lykknes



Professor, Dr.scient.
Torunn Berg



Professor, Ph.D. (London)
David Nicholson



Associate Professor, Dr.ing.
Trond Peder Flaten



Adjunct Professor
Rolf Tore Ottesen

Administrative staff



Head of administration
Lena Frostad



Senior executive officer
Lillian Hanssen



First secretary
Aase Sæther



Executive officer
Inger Marie Frøseth



Higher executive officer
Ingrid Kristine Tømmerdal



Anne Langseth

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

Alsvik, Inger Lise
Braaten, Hans Fredrik
Burheim, Odne S.
Gebremariam, Kidane Fanta
Kumelj, Tjasa
Kvalvåg, Sondre Schnell
Lervik, Anders
Lystvet, Sina Maria
Melnes, Silje
Nordløkken, Marit
Sandru, Eugenia-Mariana
Siegesmund, Øyvind
Simic, Anica
Stockmann, Vegar
Strand, Ragnhild Beate
Aaseng, Jon Erik

Demonstrators

Andersen, Marthe K.
Bakka, Thomas
Berg, Michel Brunet
Blakstad, Guro
Braadland, Peder R.
Braaten, Hans Fredrik
Bugge, Audun Nystad
Bugge, Steffen
Buraas, Ida Kristine
Draget, Ruth Sissel M.
Edwardsen, Tove-Nanny
Egede-Nissen, Cecilie
Engen, Sara Kristin H.
Engøy, Ingemund F.
Gilde, Maria
Haugland, Marius M.
Heide, Frode Sterten
Heidelberg, Cecilie T.
Helgerud, Trygve
Hellstrøm, Kaja C.
Hovde, Gunnhild
Høydal, Liv Mari B.
Høyvik, Ida-Marie
Jacobsen, Julie Berild
Johansson, Emma M.
Karlsen, Tom Rune
Kirkemo, Fredrik N.
Kjønstad, Ingrid Fadum
Kong, Xiang Yi

Demonstrators contd.

Lakså, Solveig M.B.
 Landsem, Eva
 Linde, Henrik
 Lofthus, Synnøve
 Lyngvi, Eirik
 Løvås, Jim
 Madland, Eva
 Martinsen, Morten
 McDonagh, Birgitte
 Mekki, Miriam
 Molnes, Silje Nedland
 Nauste, Kristian B.
 Nordum, Mats
 Næss, Mari Kirkebøen
 Ohm, Ragnhild
 Pedersen, Cathrine
 Ringholm, Magnus
 Rusti, Elise Hermo

Rønningen, Torunn
 Sjulstad, Eli Bjørnø
 Skorpa, Ragnhild
 Slungård, Sigrid V.
 Solvang, Tina
 Sommerseth, Camilla
 Steinsland, Synne
 Sunde, Marius
 Surdal, Cecilie
 Sørensen, Cathrine
 Sørensen, Lisbet
 Takla, Marit
 Tandberg, Paul B.
 Thvedt, Thor H. Krane
 Tungen, Jørn E.
 Tveiekrem, Marit Elise
 Yttervik, Johan Hatling
 Østensen, Ole Jørgen
 Aakre, Iselin
 Aardal, Eivind

Guest professors/researchers/lecturers

Jon Pharoah	Jan. 1 – June 30, 2009
Levent Akyalcin	Jan. 1 – Sept. 30, 2009
Sema Akyalcin	Jan. 1 – Sept. 30, 2009
Brigitte Van Tiggelen	May 7 – May 15, 2009
Marie du Toit	May 15 – June 15, 2009
Diego Fernando Mendoza Munoz	Sept.1 – Dec. 18, 2009
Vladimir Kulinskiy	Sept.17–Sept.30, 2009
Gian-Paolo Beretta	Sept.18 –Nov. 15, 2009
Helge Kragh	Oct. 14 – Oct. 17, 2009
Irina Shtangeeva	Oct. 14 – Nov. 27, 2008
Professor Peter Kjærgaard, University of Aarhus, Denmark/ University of Cambridge, Great Britain: "Et langt argument: Darwin og evolusjonsdebatten på 1800-tallet"	Sept. 14, 2009
Professor Vladimir Kulinskiy, Department of Theoretical Physics, Odessa University, Ukraine: "Kinetic and Hydrodynamic Regimes in the Dynamical Models of Self-Propelling Particles"	Sept. 21, 2009
Professor Helge Kragh, University of Aarhus, Denmark: "Aspekter av fysikkens historie I det 20. århundre"	Oct. 15, 2009
Professor Helge Kragh, University of Aarhus, Denmark: "When Cosmology became a Branch of Physics: The Period 1945-1966"	Oct. 16, 2009



Trondheim in May

Annual Report for Department of Chemistry 2009



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