

Annual Report 2014

Department of Chemistry



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From Mesocosm experiment in Patagonia (part of the EU project Ocean-Certain). Murat V. Ardelan monitoring biological and chemical variables at a cold Patagonian fjord © Jose Iriarte

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The State of the Department of Chemistry 2014

This annual report aims to give the overview of the main accomplishment for the department of chemistry in 2014 and we do hope that you find it informative and useful.

During 2014, the department continued its trend started in the previous years with a strong increase of the externally financed research projects. Some examples are given here. The Research Council of Norway (RCN) financed through the Gassmaks program, and in collaboration between the applied theoretical chemistry group and SINTEF Materials and Chemistry, a project related to chromium oxide reduction. SINTEF Materials and Chemistry is, again, our partner with the applied theoretical chemistry group in a new project financed by the RCN aiming to improve the performance of carbon insulation and refractory materials in aluminium production. The environmental and analytical chemistry group developed a project on the effects of potential leakage from sub-seabed CO₂ storage sites on the marine environment at relevant hydrostatic pressure through the Polish-Norwegian Research Program funded by EEA and Norway Grants.

We were very pleased to welcome among our technical group, staff engineer Marit Syversveen and senior engineer Anica Simic. Eva Madland is our new officer in charge of the study related matters and associate professor Ida-Marie Høyvik joined the applied theoretical chemistry group.

5 new PhD students (Elisa Magnanelli, Frank Richter, Oda Dahlen, Kristin Skjelbred and Daniel Lisø) joined us at the department of chemistry in 2014, while 8 PhD students completed and defended their dissertations (Katrine Lie Bøyesen, Apostolos Gerontas, Morten Karlsen, Svein Jacob Kaspersen, Sæpurahman, Ragnhild Skorpa, Mari Voldsund and Asma Zaidi). The department welcomed as well 3 new post-docs: Enrico Riccardi, Sondre Schnell and Anders Lervik.

Also in 2014 members of the department of chemistry were recognized for extraordinary contributions. Professor Signe Kjelstrup received the "Guldberg and Waage" medal from the Norwegian Chemical Society. She is the second lady who has ever received this prestigious prize after Professor Synnøve Liaaen Jensen. She was

acknowledged for her major contribution in irreversible thermodynamics with focus on electrochemical cells, membrane systems and energy optimization for chemical process applications. Professor Øyvind Mikkelsen was appointed from January 2014 chairman for the National Committee for Research Ethics in Science and Technology (NENT), an independent agency for questions regarding research ethics and investigation of misconduct in Science.

Increasing the quality of education at the department is a constant aspiration and activity for us. Many important accomplishments were achieved in 2014. The department is involved in several major projects granted by the rector and aiming to develop and gain experience with new and innovative teaching methods. Several members of our team are involved in the VKR project (Virtuelle Kjemiske Rom) with the objectives to improve education for General Chemistry. We are also contributing to the VfK (Video for kvalitet og fleksibilitet) and Prosjektil (Prosjekt Innovativ Lektorutdanning) projects. In 2014, several compendia for laboratory exercises have been revised and updated, and a range of actions were initiated to reduce dropout of students. In addition we were very pleased to receive funds from the rector to develop and update laboratory equipment for our basic courses. Similarly our application for a new ICP-MS has also been granted and the new equipment dedicated for instrumental multi-element analysis of the composition of a wide variety of materials will be purchased in 2015.

*Marie-Laure Olivier
Head of Department*

(R)-Stiripentol, an anti-epileptic drug

Enantiopure drugs

It is well known that enantiomers of a racemic drug may have different pharmacokinetic and pharmacodynamic effects. The body will interact with and metabolise each enantiomer differently to produce different pharmacological activities.

Thus, one isomer (eutomer) may produce the desired therapeutic activities, while the other (distomer) may be inactive or, in worst cases, produce unwanted negative effects. (Sheldon, 1993) US Food and Drug Administration (FDA) considers one enantiomer (distomer) as an impurity of the other enantiomer (eutomer). This requires independent investigations of both enantiomers of chiral drugs. Therefore, development of new analytical and preparative techniques to obtain pure enantiomers has become of particular importance for pharmaceutical industry. (Collins *et al.*, 1992; Collins *et al.*, 1997)

Stiripentol - an anti-epileptic drug

Stiripentol, *rac*-1-(benzo[d][1,3]dioxol-5-yl)-4,4-dimethylpent-1-en-3-ol (*rac*-1) is a novel anti-epileptic drug structurally unrelated to any other anti-epileptic drugs. It has been suggested that stiripentol induced increase in gamma amino butanoic acid (GABA) concentration through at least two independent neurochemical mechanisms. (Trojnar *et al.*, 2005)

Epilepsy

Epilepsy is a central nervous system pathology characterised by seizures. The disease is treated by several drugs, f. inst acetazolamide, clonacepam, carbamazepine, pregabalin, clobazam and valproate. Stiripentol is used mostly for children treatment. Several of the above mentioned drugs act on the gamma aminobutyric acid receptor (GABA). This is the receptor in the brain where the most common inhibitory synapses are regulated. (Figure 1) It is known that epilepsy patients may have mutations in the GABA_A receptor.

Recently, it was reported that stiripentol acts directly on the GABA_A receptor as a positive allosteric modulator. (Fischer *et al.*, 2009) In addition, its anticonvulsant potency had been proven in different types of animal seizures, as well as in clinical trials. (Chiron, 2005) Stiripentol is a secondary alcohol containing one stereogenic center. So far, it is marketed as a racemic mixture, albeit, there are marked differences in pharmacokinetics and antiepileptic potency between the enantiomers. (Trojnar *et al.*, 2005)

Resolution by biocatalysis

Resolution is one of the major strategies for providing enantiopure chiral building blocks (CBB's) for drug synthesis. Enzyme catalysed kinetic resolution is a common method in order to obtain

CBB's. Enzymes are remarkable catalysts, capable of accepting a wide range of substrates, at the same time exhibiting chemo- regio-, and enantioselectivity. (Fessner and Anthonson, 2009; Bommarium and Riebel, 2004) Hydrolytic enzymes, in particular lipases, are most commonly used as biocatalysts for enzymatic resolution. Most lipases accept a broad range of non-natural substrates and are thus very versatile for applications in organic synthesis. They do not require cofactors and are commercially available in free and immobilised forms. In many cases, they exhibit good to excellent stereoselectivity.

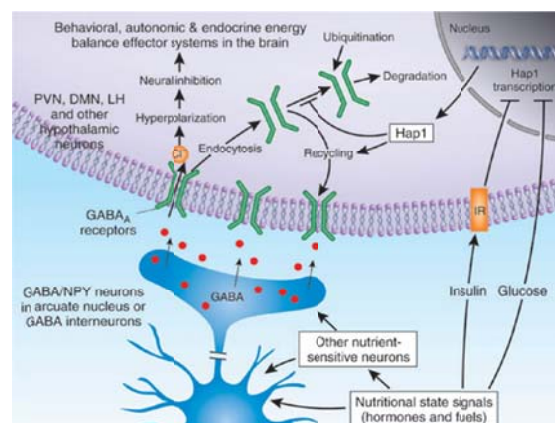
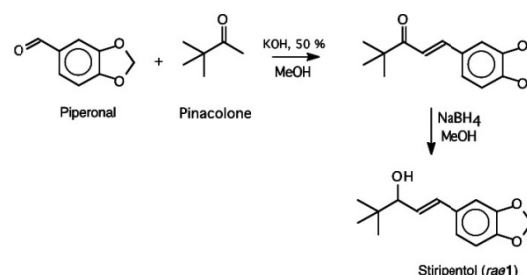


Figure 1. Gamma aminobutyric acid receptors, GABA.

(R)-Stiripentol in 94 % ee

Stiripentol (*rac*-1) was prepared in good yields from piperonal and pinacolone followed by reduction using sodium borohydride. (Scheme 1) (Vallet, 1975)



Scheme 1. Synthesis of stiripentol (1) from piperonal and pinacolone.

The racemic alcohol **1** was resolved using vinyl butanoate in hexane and catalysed by Lipase A from *Candida antarctica* (CALA). (Scheme 2) (Jacobsen *et al.*, 2012) Several lipases were tested for the reaction, but as expected, CALA was the best catalyst. (Kirk *et al.*, 2002) CALA is in the collection of lipases, which exhibit strong restriction on the acid part having a narrow tunnel to accommodate the acyl group, but a wider alcohol binding site. (Naik *et al.*, 2010)

Chiral analyses and optical rotation

The secondary alcohol, (3*R*)-1, produced by CALA catalysed hydrolysis of the produced butanoate had optical rotation $[\alpha]_D +23.9$ (c 10 CHCl₃) for 94% ee. Hence, the absolute configurations of the faster reacting enantiomer was established as being (*R*) since it has been reported that (*R*)-stiripentol has specific optical rotation $[\alpha]_D +24.9$ (c 2.61 MeOH). (Zhang *et al.*, 1994) The slower reacting alcohol (*S*)-1, showed $[\alpha]_D -18.1$ (c 10 CHCl₃) for 86% ee. The (*R*)-butanoate, (*R*)-2, eluted as the second isomer in chiral HPLC (Chiralcel OD-H column) as compared to the (*R*)-alcohol, which was the first eluted enantiomer (Figure 2). Also, it showed levorotatory effect $[\alpha]_D -68.0$ for 92% ee, whereas the (*R*)-alcohol has a dextrorotatory effect.

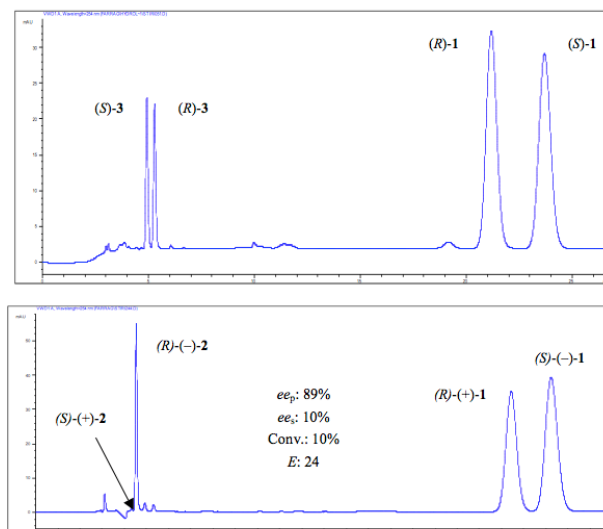
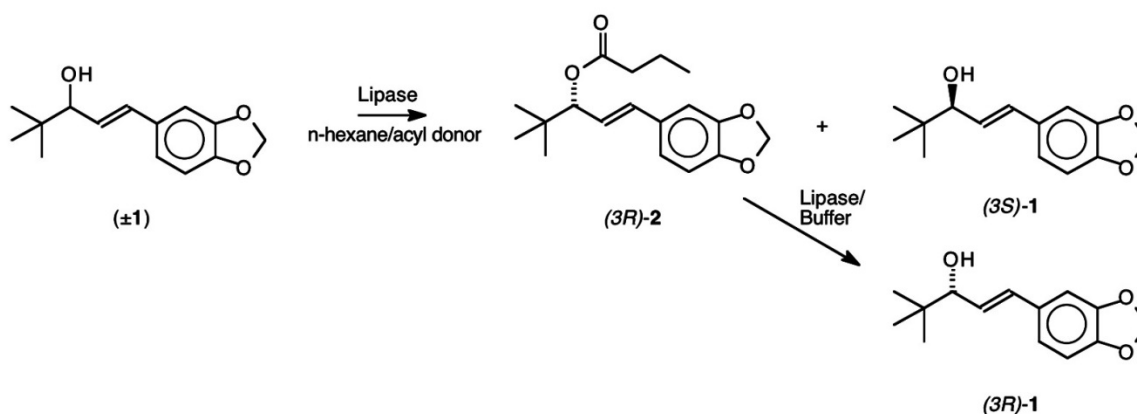


Figure 2. HPLC analyses of enantiomers of stiripentol (1), stiripentol butanoates (2) and stiripentol acetates (3).



Scheme 2. Lipase catalysed esterification of stiripentol (1) with subsequent lipase catalysed hydrolysis of (*R*)-stiripentol butanoate ((3*R*)-2) to (*R*)-stiripentol ((3*R*)-1) in 94 % ee.

Acknowledgements

The project was funded by The Research Council of Norway (contract Grant Number 202903/11).

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Elisabeth Jacobsen

Hvordan ville en nanoskopisk smultring ha smakt?

En nanometer er en milliontedels millimeter, det vil si veldig smått. En nanometer i forhold til en meter kan sammenlignes med størrelsen på en klinkekule i forhold til hele jordkloden. Til tross for den beskjedne størrelsen, spår direktør ved NTNUs Nanolab, Kay Gastinger, at nanoteknologi kommer til å bli Norges framtidsnæring når oljen tar slutt.[1] Nanoteknologi gjør det mulig å skape nye stoffer og gjenstander med superegenskaper. Et eksempel er de utrasterke nano-karbonrørene, som i framtiden kan gjøre det mulig å bygge heis ut i verdensrommet.[2] Det forskes også på nanoroboter som vil kunne levere cellegift direkte til kreftcellene, og dermed spare pasienter for mye lidelse. Men vi forstår ikke helt hvordan ting oppfører seg på nanonivå. Vi vet at ting er annerledes enn på makronivå, hvor vi lever. Noe av utfordringen ligger i at ting er for smått til å beskrives av fysikkens klassiske teorier som gjelder på makronivå, og for stort til å beskrives av enkle atommodeller.

Overflatene til nanoskopiske objekter spiller en nøkkelrolle for deres egenskaper. Hvis du ser på overflaten i en kaffekopp, ser den for oss ut som en brå overgang mellom luft og kaffe. Hadde man zoomet inn til nanonivå, ville man sett en veldig smal region på kanskje 1-2 nanometer, den såkalte «overflateregionen», med egenskaper forskjellige fra både luften og kaffen.

Det er denne overflateregionen som gjør at det kan være meget smertefullt å ta mageplask fra stupebrettet. Siden overflateregionen er såpass smal, utgjør den en liten del av svømmebassenget som helhet, og man merker den sannsynligvis kun etter ett uheldig stup. For nanoskopiske objekter derimot, vil overflateregionen utgjøre en betydelig del på grunn av deres beskjedne størrelse. Her i forskningsgruppen for ikke-likevekts termodynamikk ved NTNU prøver vi å forstå hva som skjer i denne overflateregionen, og hvordan dens egenskapene kan utnyttes både i dagens og i framtidens teknologi.



Nanoskopiske objekter vil kunne ha helt spesielle egenskaper avhengig av deres form og fasong. En nanopartikkel med smultringform, vil for eksempel ta til seg og videreføre varme på en helt annen måte enn en nanopartikkel med dråpeform, selv om de er laget av samme materiale. Dette skyldes overflatekrumningen til den lille nanosmultringen. I vår faggruppe har vi utviklet en ny beregningsmetode for å finne ut av nettopp hvordan formen påvirker disse egenskapene.[3] Metoden kombinerer informasjonen fra atomistiske simuleringer, der man simulerer hvordan partiklene vekselvirker med hverandre, med en matematisk beskrivelse av overflateregionen.

Se for deg at vi ønsket å steke noen smultringer til kaffen. Gitt at temperaturen i stekeovnen var den samme overalt, ville vanlige smultringer etter all sannsynlighet bli jevnt stekt og smake fortreffelig. Hvis vi skulle stekt en nanoskopisk smultring i den samme ovnen, ville den sterke krumningen gjøre at den ble svidd på utsiden, men deigete på innsiden. Selv om dette er en ulempe for smultringer, kan vi altså gi nano-objekter helt spesielle egenskaper ved å spesialtilpasse deres form og fasong.

Vi ser for oss at vår beregningsmetode for å regne ut hvordan fasongen påvirker egenskapene, vil kunne ha mange forskjellige bruksområder. Den kan for eksempel tas nytte av i design av framtidens datamaskiner for å lettere transportere ut varme, og dermed gjøre det mulig å øke prosessorkraften.

Research Projects

Et annet mulig bruksområde er i utviklingen av selvdrivne nanopartikler for å levere medisin direkte til det syke organet i kroppen. Det første målet vårt er å bruke metoden for å utvikle mer presise modeller for hvor kjapt væsker fordampes og gasser kondenserer. Når kaffen koker i kaffetrakten, eller dugg kondenserer på vindusruten, starter denne prosessen med bittesmå nanoskopiske bobler og dråper. Nettopp i denne fødselsprosessen for boblene og dråpene, vil de være nanoskopiske og ha lignende særegenheter som nanosmultringen. Ved å forstå disse særegenhetene forventer vi å kunne beskrive lignende prosesser i industrien mer presist, for eksempel i kokere eller destillasjonskolonner, og gjøre det mulig å lage mindre og mer effektivt prosessutstyr. I årene som kommer tror vi at satsing på grunnleggende forskning er nøkkelen for bane vei for teknologiske nyvinninger innenfor nanoteknologi, å slik gjøre Norge til en ledende nasjon innen nanoteknologi når oljen tar slutt. Det er mange fantastiske muligheter som venter på å bli oppdaget innenfor dette spennende fagfeltet.

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Beskrivelse av meg:

Øivind Wilhelmsen er doktorgradsstipendiat i ved Institutt for Kjemi på NTNU, og er også forsker i SINTEF Energi. Han forsker på termodynamikk og kjemisk fysikk for overflater og jobber med å lage matematiske beskrivelser av prosesser både i naturen og industrien for å forstå de bedre.

Scientific Publications

Applied Theoretical Chemistry

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Antarctic ocean@M.Ardelan

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Murat Ardelan in his home-made clean room onboard the research vessel in Antarctica ©M. Ardelan

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B. Alsberg

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F. Bresme

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A. Fiksdahl

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NTNU's board member of "Anders Jahres Fond" (2010 -).

Member of expert committee, Frinatek, The Research Council of Norway.

Secretary of board, the Group of Organic Chemistry of the Norwegian Chemical Society.

Board member, "Lundgrens enkes fond", NTNU.

Board member at Department of Chemistry, NTNU.

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T.P. Flaten

Editor, Norsk Epidemiologi ((Norwegian Journal of Epidemiology).

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

Board member, Norwegian Chemical Society, Trondheim Branch.

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

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Activities

O.R. Gautun

Section leader, Organic chemistry group, Department of chemistry, NTNU.

Member of expert committee for risk assessment, Department of chemistry, NTNU.

Member of NFR's (Norwegian research council) committee for marine bioprospecting and organic synthesis.

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K.F. Gebremariam

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B. Hafskjold

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J. Han

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E. Hjertenæs

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B.H. Hoff

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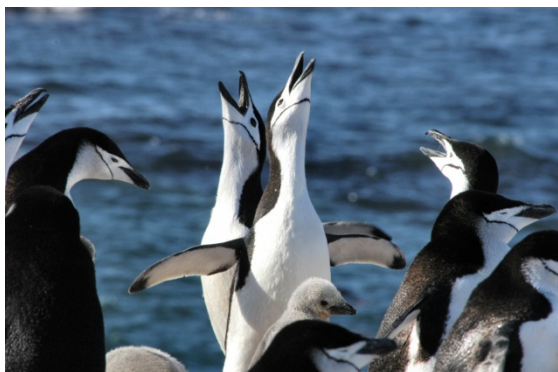
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Barren landscape by the old whaling station ©M.Ardelan

N. Iqbal

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Crying penguins ©M.Ardelan

E. Jacobsen

Scientific committee member, European Federation of Biotechnology, Section on Applied Biocatalysis.

Editorial Board member, Biocatalysis and Biotransformation, Taylor & Francis.

Working group member and Management committee member (deputy), COST Action CM1303, Systems Biocatalysis.

Reviewer for one or more manuscripts in the following scientific periodicals: *Energies*, *Journal of Biotechnology*, *Journal of Molecular Catalysis B: Enzymatic*, *Biocatalysis and Biotransformation*, *Enzyme engineering*, *International Journal of Chemistry and Materials Research*, *International Journal of Medicinal and Pharmaceutical Case reports*.

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S.J. Kaspersen

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S. Kjelstrup

Member of PHYCHEMA Group, Science Europe, Brüssel.

Receiver of the "Guldberg and Waage" medal by NKS (Norwegian Chemical Society) at the 20th National meeting in Lillestrøm, Norway, 29.11.2014.

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An old grave at the Deception Island ©M.Ardelan

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L. Kvittingen

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A. Lykknes

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E. Madland

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K. Mathisen

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Ø. Mikkelsen

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R. H. Myhre

Skjelbred, Kristin Marie; Myhre, Rolf Heilemann; Koch, Henrik; de Merás, Alfredo Sánchez. MLCC - Multi Level Coupled Cluster Theory. Norsk kjemisk selskaps landsmøte; 2014-10-29 - 2014-10-30.

M.- L. Olivier

Head of the Department of Chemistry.



Seals ©M.Ardelan

V. Partali

Member of the department's approval committee for students' master degree plans.

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N. Sanchez

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R. Schmid

Section leader, environmental and analytical chemistry group, Department of chemistry, NTNU.

Member of the department's approval committee for students' master degree plans.

Bukhari, Syed Majid; Feuerherm, Astrid Jullumstrø; Tunset, Hanna Maja; Isaksen, Stian Moe; Sæther, Mari; Thvedt, Thor Håkon Krane; Gonzalez, Susana V.; Schmid, Rudolf; Fuglseth, Erik; Zlatkovic, Bojan; Johansen, Berit; Simic, Nebojsa. Sclerochloa dura: A new source of anti-inflammatory compounds. 13th national NMR Meeting; 2014-01-14 - 2014-01-15.

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A. Simic

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E. Steinnes

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G.M. Tesfamariam

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Trinh, Thuat; Bedeaux, Dick; Kjelstrup, Signe. Prediction of Chemical Potential and Activity Coefficient of Graphite Surface from Molecular Dynamics Simulation. International Conference on Computational Science and Technology 2014 (ICCST2014), Polen; 2014-05-15 - 2014-05-16.

Trinh, Thuat; Bedeaux, Dick; Kjelstrup, Signe; van Erp, Titus Sebastiaan; Nagel, Henrik Rojas; Holvik, Egil. Thermodynamics of CO₂ adsorbed on a graphite surface. Lorentz Workshop: Nanothermodynamics: For Equilibrium and Non-Equilibrium, Leiden, Netherlands; 2014-12-01 - 2014-12-05.

Trinh, Thuat; Kjelstrup, Signe; Bedeaux, Dick. Thermal conductivity of carbon dioxide from non-equilibrium molecular dynamics. Det 20 landmøte i Kjemi, Lillestrøm, Norge; 2014-10-29 - 2014-10-30.

Trinh, Thuat; Vlugt, Thijs J.H.; Hagg, May-Britt; Bedeaux, Dick; Kjelstrup, Signe. Simulation study of pore size and charge effect to the selectivity of CO₂/H₂ syngas mixture in a carbon membrane. 3rd Trondheim Gas Technology Conference (TGTC-3), Trondheim, Norge; 2014-06-04 - 2014-06-05.

Wilhelmsen, Øivind; Trinh, Thuat; Kjelstrup, Signe; Bedeaux, Dick. Heat and Mass Transfer across Interfaces in Complex Nano-Geometries. Lorentz workshop: Nanothermodynamics: For Equilibrium and Non-Equilibrium, Leiden, Netherlands; 2014-12-01 - 2014-12-05.

T. van Erp

Trinh, Thuat; Bedeaux, Dick; Kjelstrup, Signe; van Erp, Titus Sebastiaan; Nagel, Henrik Rojas; Holvik, Egil. Thermodynamics of CO₂ adsorbed on a graphite surface. Lorentz Workshop: Nanothermodynamics: For Equilibrium and Non-Equilibrium, Leiden, Netherlands; 2014-12-01 - 2014-12-05.

van Erp, Titus Sebastiaan. On the relation between the Langmuir and thermodynamic flux equations. Lorentz workshop: Nanothermodynamics, For Equilibrium and Non-Equilibrium; 2014-12-01 - 2014-12-05.

van Erp, Titus Sebastiaan. Reaction rate calculation using path sampling: pitfalls and opportunities. talk; 2014-07-07 - 2014-07-11.

V. Venkatraman

Abburu, Sailesh; Venkatraman, Vishwesh; Foscatto, Marco; Jensen, Vidar Remi; Alsberg, Bjørn Kåre. A de novo design approach to enhance the optical properties of azobenzenes. Swedish Theoretical Chemistry Meeting 2014; 2014-10-27 - 2014-10-29.

Alsberg, Bjørn Kåre; Venkatraman, Vishwesh; Gupta, Mayuri; Foscatto, Marco; Svendsen, Hallvard Fjøsne; Jensen, Vidar Remi. Evolutionary de novo design of absorbents for CO₂ capture. Swedish Theoretical Chemistry Meeting 2014; 2014-10-27 - 2014-10-29.

Foscatto, Marco; Occhipinti, Giovanni; Venkatraman, Vishwesh; Alsberg, Bjørn Kåre; Jensen, Vidar Remi. Automated Design of Organometallic Compounds from 3D Fragments. 5th EuCheMS Chemistry Congress; 2014-08-31 - 2014-09-04.

Foscatto, Marco; Occhipinti, Giovanni; Venkatraman, Vishwesh; Alsberg, Bjørn Kåre; Jensen, Vidar Remi. Automated in Silico Design of Homogeneous Catalysts. 19th International Symposium on Homogeneous Catalysis; 2014-07-06 - 2014-07-11.

S. Villa Gonzalez

Sandru, Eugenia-Mariana; Sielk, Jan; Burghaus, Jens; Øpstad, Christer L.; Simic, Nebojsa; Gonzales, Susana Villa; Sliwka, Hans-Richard; Partali, Vassilia. Thiocarbonyl polyenes: monomers, trimers, and thiopyrans. The 13th National MR Meeting; 2014-01-14 - 2014-01-15.

Ø. Wilhelmsen

Bedeaux, Dick; Wilhelmsen, Øivind; Kjelstrup, Signe; Glavatskiy, Kirill. Curvature dependence of the heat and mass transfer resistances of the surface of nano bubbles and droplets. The 5th Nordic Workshop on Statistical Physics: Biological, Complex and Non-Equilibrium Systems, Stockholm, Sweden; 2014-03-26 - 2014-03-28.

Bedeaux, Dick; Wilhelmsen, Øivind; Kjelstrup, Signe; Glavatskiy, Kirill. Curvature dependence of the heat and mass transfer resistances of the surface of nano bubbles and droplets. Computational condensed matter: advances and challenges, Whitehaven, UK; 2014-09-08 - 2014-09-09.

Bedeaux, Dick; Wilhelmsen, Øivind; Kjelstrup, Signe; Glavatskiy, Kirill. Curvature dependence of the heat and mass transfer resistances of the surface of nano bubbles and droplets. 27th European Symposium on Applied Thermodynamics, Eindhoven, Netherlands; 2014-07-06 - 2014-07-09.

Magnanelli, Elisa; Wilhelmsen, Øivind; Johannessen, Eivind; Kjelstrup, Signe. Modelling of membrane units for CO₂ separation with Non-Equilibrium Thermodynamics. 27th European Symposium on Applied Thermodynamics; 2014-07-06 - 2014-07-09.

Wilhelmsen, Øivind; Bedeaux, Dick; Kjelstrup, Signe. Heat and Mass Transfer through Interfaces of Nanosized Bubbles and Droplets. ETH Polymer Physics Seminars, Zürich, Switzerland; 2014-05-07 - 2014-05-07.

Wilhelmsen, Øivind; Trinh, Thuat; Kjelstrup, Signe; Bedeaux, Dick. Heat and Mass Transfer across Interfaces in Complex Nano-Geometries. Lorentz workshop: Nanothermodynamics: For Equilibrium and Non-Equilibrium, Leiden, Netherlands; 2014-12-01 - 2014-12-05.

Zlotorowicz, Agnieszka; Burheim, Odne Stokke; Strand, Robin Viktor; Wilhelmsen, Øivind; Kjelstrup, Signe. The impact of the water transference number on the permselectivity of ion exchange membranes and reverse electrodialysis. Second International Conference on Salinity Gradient Energy; 2014-09-10 - 2014-09-12.

A. Zlotorowicz

Zlotorowicz, Agnieszka; Burheim, Odne Stokke; Strand, Robin Viktor; Wilhelmsen, Øivind; Kjelstrup, Signe. The impact of the water transference number on the permselectivity of ion exchange membranes and reverse electrodialysis. Second International Conference on Salinity Gradient Energy; 2014-09-10 - 2014-09-12.

Zlotorowicz, Agnieszka; Sunde, Svein; Seland, Frode. Modification of the Oxygen Evolution Catalytic Layer with Zirconium(IV) Hydrogenphosphate. International Symposium on Electrocatalysis: Explorations of the Volcano Landscape; 2014-10-26 - 2014-10-29.

P. – O. Åstrand

Leader (elected), Division of Computational Chemistry, Norwegian Chemical Society (2010-). Member, National Domain-specific Committee for Chemistry, NOTUR, Uninett (2013-).

Lecturer, Summer school on Molecular Dynamics and Chemical Kinetics, Copenhagen, August 2014.

Daub, Christopher David; Åstrand, Per-Olof; Österberg, Ulf Lennart; Bresme, Fernando. Molecular reorientation in fluids resulting from thermal gradients. 248th American Chemical Society National Meeting; 2014-08-10 - 2014-08-14.

Davari, Nazanin; Daub, Christopher David; Åstrand, Per-Olof; Unge, Mikael. Atomistic simulations of the local electric field in dielectric liquids. 2014 IEEE International Conference on Liquid Dielectrics; 2014-06-30 - 2014-07-03.

Davari, Nazanin; Åstrand, Per-Olof; Unge, Mikael. Field-dependent ionization potential for polyaromatic molecules from constrained density-functional theory. 2014 IEEE International Conference on Liquid Dielectrics; 2014-06-30 - 2014-07-03.

Haghdani, Shokouh; Davari, Nazanin; Åstrand, Per-Olof. The $\pi \rightarrow \pi^*$ Excitation Energy of Azo Compounds by a Combined Charge-Transfer and Point-Dipole Interaction Model. Det 20. Landsmøte i Kjemi; 2014-10-29 - 2014-10-30.

Åstrand, Per-Olof. Electrical insulation in dielectric liquids: a case for quantum chemistry?. Mini symposium; 2014-09-12.

Åstrand, Per-Olof. Improved liquids for electrical insulation: a case for quantum chemistry?. Guest lecture; 2014-08-14.

Åstrand, Per-Olof. New liquids for electrical insulation: a case for quantum chemistry? Guest lecture; 2014-05-12.

Graduate Students

Spring examination

Course no.	Course title (credits)	Lectures and exercise coordinators	Candidates/Passed
KJ1020	Organic Chemistry (15)	Vassilia Partali	123/104
KJ1042	Basic Thermodynamics with Laboratory (7,5)	Signe Kjelstrup	104/94
KJ2022	Spectroscopic Methods in Organic Chemistry (7,5)	Nebojsa Simic	33/24
KJ2031	Inorganic Chemistry, Advanced Course	Karina Mathisen	6/6
KJ2053	Chromatography (7,5)	Rudolf Schmid	40/38
KJ2072	Environmental Chemistry (7,5)	Torunn Berg	38/33
KJ2073	Analytical Environmental Chemistry (7,5)	Øyvind Mikkelsen Trond Peder Flaten	19/19
KJ2095	Experts in Teamwork - Environmental Influences on Human Health (7,5)	Trond Peder Flaten	22/22
KJ6003	Basic Organic chemistry (Kompis)	Lise Kvittingen	6/6
KJ8056	Chemical and Sensors and Biosensors	Florinel-Gabriel Banica	2/2
KJ8209	Application of Advanced Chemometric Methods	Viswesh Venkatraman	3/3
TKJ4130	Organic Synthesis, Laboratory (7,5)	Vassilia Partali Bård Helge Hoff	9/9
TKJ4135	Organic Synthesis, Advanced Course (7,5)	Anne Fiksdahl	4/4
TKJ4150	Organic Synthesis I (7,5)	Bård Helge Hoff Anne Fiksdahl	32/19
TKJ4170	Quantum Chemistry (7,5)	Titus van Erp	10/10
TKJ4175	Chemometrics(7,5)	Bjørn Kåre Alsberg	8/8
TKJ4215	Statistical Thermodynamics in Chemistry and Biology (7,5)	Per-Olof Åstrand	35/29
TKJ4510	Physical Chemistry, Specialization Project (15)	Bjørn Kåre Alsberg	
TKJ4520	Organic Chemistry, Specialization Project (15)	Odd Reidar Gautun	

Autumn examination

Course no.	Course title (credits)	Lectures and exercise coordinators	Candidates/Passed
KJ1000	General Chemistry (15)	Bjørn Hafskjold	201/188
KJ1041	Chemical Bond, Spectroscopy and Kinetics (7,5)	Ida-Marie Høyvik	138/122
KJ2050	Analytical Chemistry, Basic Course (7,5)	Øyvind Mikkelsen	71/66
KJ3021	Nuclear Magnetic Resonance Spectroscopy	Nebojsa Simic	20/19
KJ3022	Spectroscopic Methods in Organic Chemistry, Advanced Course (7,5)	Nebojsa Simic	1/1
KJ3050	Marine Organic Environmental Chemistry (7,5)	Øyvind Mikkelsen	12/12
KJ3051	Ocean space: Marine Geochemical Processes	Murat van Ardelan	7/7
KJ3053	Analytical Methods for Industrial- and Environmental Monitoring (7,5)	Bjørn Kåre Alsberg Florinel Gabriel Banica	5/5
KJ3059	Chromatography, Advanced Course	Rudolf Schmid	9/6
KJ3071	Applied Geochemistry (7,5)	Rolf Tore Ottesen	12/12
KJ3072	Advanced Aquatic Chemistry (7,5)	Trond Peder Flaten	14/14
KJ8059	Chromatography, Advanced Course	Rudolf Schmid	2/1
KJ8072	Advanced Aquatic Chemistry (7,5)	Trond Peder Flaten	2/2
KJ8107	New Concepts in Organic Synthesis	Bård H. Hoff	4/4
KJ8205	Advanced Molecular Modelling	Per-Olof Åstrand	7/7
KJ8902	Molecular Modelling (7,5)	Titus van Erp	2/2
KJ8903	Irreversible Thermodynamics (7,5)	Signe Kjelstrup	5/5
TKJ4102	Basic Organic Chemistry	Elisabeth Egholm Jacobsen	124/101
TKJ4155	Organic Synthesis II	Anne Fiksdahl	11/9
TKJ4180	Physical Organic Chemistry (7,5)	Odd Reidar Gautun	19/16
TKJ4200	Irreversible Thermodynamics (7,5)	Signe Kjelstrup	7/7
TKJ4205	Molecular Modelling (7,5)	Titus van Erp	12/12
TKJ4510	Physical Chemistry, Specialization Project (15)	Bjørn Kåre Alsberg	
TKJ4520	Organic Chemistry, Specialization Project (15)	Odd Reidar Gautun	8/8
TKJ4525	Organic Chemistry, Specialization Course (7,5)	Anne Fiksdahl	1/1

Graduate Students

Re-sit examination

Course no.	Course title (credits)	Candidates/Passed
RFEL1001	Natural Science and World Views (7,5)	
KJ1000	General Chemistry (15)	16/14
KJ1020	Organic Chemistry (15)	3/0
KJ1041	Chemical Bond Theory and Spectroscopy (7,5)	7/6
KJ1042	Basic Thermodynamics with Laboratory (7,5)	12/10
KJ2022	Spectroscopic Methods in Organic Chemistry (7,5)	1/1
KJ2050	Analytical Chemistry, Basic Course (7,5)	1/1
KJ2053	Chromatography (7,5)	1/1
KJ2072	Environmental Chemistry (7,5)	1/1
KJ2073	Analytical Environmental Chemistry (7,5)	3/3
KJ3021	Nuclear Magnetic Resonance Spectroscopy (7,5)	
KJ3022	Spectroscopic Methods in Organic Chemistry, Advanced Course (7,5)	2/1
KJ3050	Marine Organic Environmental Chemistry (7,5)	
KJ3053	Analytical Methods for Industrial- and Environmental Monitoring (7,5)	
KJ8059	Chromatography, Advanced Course	
TKJ4102	Basic Organic Chemistry(7,5)	
TKJ4135	Organic Synthesis, Advanced Course (7,5)	9/6
TKJ4150	Organic Synthesis I (7,5)	
TKJ4170	Quantum Chemistry (7,5)	1/1
TKJ4175	Chemometrics (7,5)	
TKJ4180	Physical Organic Chemistry	
TKJ4190	Physical Chemistry, Project Work (7,5)	1/0
TKJ4215	Statistical Thermodynamics in Chemistry and Biology (7,5)	3/2



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Siv.ing. students

3. year (MTKJ)

Adnan, Mohammed Mostafa
 Hansen, Sondre Kværne
 Johansen, Camilla
 Myreng, Kristian Njerve
 Ose, Eline Ekorholm
 Strandheim, Kristine Olsen
 Sundby, Kristin
 Sæther, Sandra
 Tvedten, Klara Elisabeth
 Trommestad, Trym Christian
 Vold, Martin Furru
 Wæhle, Morten Nasset

4. year (MTKJ)

Aae, Bjørn Erik Sylthe
 Falck, Merete
 Folkestad, Sarai Dery
 Fougner, Hugo In'T Veld
 Kjønstad, Eirik Fadum
 Kringhaug, Henrik Holthe
 Haarseth, Pia Kristine
 Hereide, Yngve Mannsåker
 Larsen, Kristin Uhlving
 Lindberg, Daniel
 Nguyen, Phuong Toan
 Reiersølmoen, Ann Christin
 Roest, Didrik Lindberg
 Uggerud, Nora
 Walderhaug, Martin E.

5. year (MTKJ)

Asplin, Alexander
 Bekkevard, Pål Unnerud
 Buene, Audun Formo
 Evjen, Sigvart
 Hansen, Ole Kudsk
 Henriksen, Silje
 Landsem, Elise
 Lund, Ingvild Teigen
 Ringheim, Ingvild

Master students in progress

Master in chemistry (MKJ)

Ali, Daniel
 Benden, Tonje Fagertun
 Berge, May-Britt
 Fauskanger, Tine Olsen
 Finstad, Martin
 Haugen, Ingrid Naterstad
 Hirkjølen, Morten
 Nervik, Sondre
 Prydz, Halvor
 Simensen, Jan Tore
 Sjursen, Kenneth Røsvik
 Tveit, Erik Våland
 Williamsen, Fredrik Bysting

Master in chemistry (MSCHEM)

Aarøen, Ola
 Amundsen, Filip
 Brondz, Anton
 Buvik, Vanja
 Bøckmann, Pål Lønnegraff
 Eriksen, Nora Meling
 Kristoffersen, Simeon
 Lea, Kristoffer Larsen
 Rian, Johan Kolseth
 Stakvik, Linda

Master in environmental chemistry (MSENVITOX)

Belay, Masho Hilawie
 Dunnebier, Dorien A. E.
 Halbach, Katharina
 Hammer, Hilde Alida
 Johanssen, Tony Helmersen
 Lee, SaeMi
 Myrstad, Marie
 Stankova, Radka
 Wang, Pan

Master of science education (MLREAL)

Berg, Håvard
 Espelien, Karoline
 Hole, Inger Ane
 Hopland, Eivind Rykkje
 Kveli, Sigrid Myhr
 Kvitrud, Kristin
 Slenes, Mari Moen

Post Graduate Students

The following Ph.d. projects are in progress

PhD-student	Working title	Supervisors
Abburu, Sailesh	Development and use of de novo design tools to find new transition metal complexes with optimal properties.	Alsberg, Bjørn K. (main superv.) Jensen, Vidar R
Badina, Aderonke	Efficient production of fuels from biomass- The use of microwave and hydrolic enzymes in processing of biomass.	Hoff, Bård Helge
Bakka, Thomas A	Synthesis of novel antibiotics inspired by marine natural products	Gautun, Odd R. (main superv.) Strøm, Morten Bøhmer Fiksdahl, Anne
Bugge, Steffen	Heteroaromatic compounds as new anticancer agents, diagnostic tools, and protozoal agents	Hoff, Bård Helge
Børset, Marit Takla	Methods to utilize waste heat in the ferro alloy industry	Kjelstrup, Signe (main superv.) Burheim, Odne Kolbeinsen, Leiv
Catelli, Emilio	Norwegian cultural heritage: A chemical perspective	Banica, Florinel (main superv.) Kvittingen, Lise
Dahlen, Oda	Studying biological transitions and aqueous phase reactions using rare event simulation techniques	van Erp, Titus (main superv.) Høyvik, Ida-Marie
Davari, Nazanin	Molecular modeling of breakdown processes in electrically insulating liquids	Åstrand, Per-Olof (main superv.) Ingebrigtsen, Stian
Forselv, Stian	Catalytic conversion of 2nd generation biomass to liquid fuels over nanostructured hierarcial solids	Mathisen, Karina (main superv.) Svelle, Stian Bjørngen, Morten
Gebremariam, Kidane Fanta	Analytical methods for art objects investigation	Kvittingen, Lise (main superv.) Banica, Florinel
Haghdani, Shokouh	Force field model for optical rotation in macromolecules	Åstrand, Per-Olof (main superv.) Alsberg, Bjørn K. Koch, Henrik
Han, Jin	Identification of TIE2 inhibitor for cancer treatment	Hoff, Bård H. (main superv.) Sundby, Eirik
Hjertenæs, Eirik	Quantum chemical calculations on sodium-graphite systems and development of a computational method utilizing non-orthogonal Slater Determinants	Koch, Henrik (main superv.) Andersson, Stefan

PhD-student	Working title	Supervisors
Iftekhar, Shafia	Trace metals and natural organic matters in rivers	Berg, Torunn (main superv.) Flaten, Trond Peder Mikkelsen, Øyvind
Lisø, Daniel	Molecular modelling of piezoelectric materials	Åstrand, Per-Olof (main superv.) Einarsrud, Mari-Ann Selbach, Sverre Magnus
Løkken, Torbjørn Vegard	Analyser av vannduggpunkt og hydrokarbonduggpunkt i naturgass. (Determination of water dewpoint and hydrocarbon dewpoint in natural gas.)	Schmid, Rudolf (main superv.) Fredheim, Arne Olav
Magnanelli, Elisa	The state of minimum entropy production of membrane processes for enhanced oil/gas recovery	Kjelstrup, Signe (main superv.) Johannessen, Eivind
Mahmoodinia, Mehdi	Molecular modelling of the Fischer-Tropsch process	Åstrand, Per-Olof (main superv.)
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	Mikkelsen, Øyvind (main superv.) Schmid, Rudolf
Moqadam, Mahmoud	Studying silica oligomerization reactions using QuantIS	van Erp, Titus Åstrand, Per-Olof
Myhre, Rolf Heilemann	Development and implementation of multi-level coupled cluster methods	Koch, Henrik (main superv.) Sunde, Svein
Nordløyken, Marit	Trace of elements in Norwegian deer	Berg, Torunn (main superv.) Flaten, Trond Peder Steinnes, Eiliv
Puerto, Nicolas Sanchez	Iron bioavailability to phytoplankton and its feedbacks to the biogeochemical cycling in the Mediterranean and Polar ecosystems	van Ardelan, Murat (main superv.) Olsen, Yngvar
Raju, Rajesh	Optically active amphiphiles and artificial cells	Gautun, Odd Reidar
Richter, Frank	Heat and life in lithium-ion secondary batteries	Kjelstrup, Signe (main superv.) Burheim, Odne Vie, Preben
Siah, Huey-San Melanie	Gold catalysis in organic synthetic chemistry	Fiksdahl, Anne (main superv.) Gautun, Odd Reidar
Simic, Anica	Trace elements and persistent organic pollutants (POPs) in blood serum samples from the Nord-Trøndelag health study (HUNT) and the possible role of trace elements in type 2 diabetes	Flaten, Trond P. (main superv.) Midtjell, Kristian

Post Graduate Students

PhD-student	Working title	Supervisors
Skjelbred, Kristin	Reduction of chromium oxide and chromite ores by methane – a computational chemistry study	Åstrand, Per-Olof (main superv.) Støvneng, Jon Andreas Andersson, Stefan
Tesfamariam, Gebrekidan M.	Enhancing the quality and relevance of chemistry teacher training education in Ethiopia: A study of the use and impact of small-scale, low cost experiments at Mekelle University	Lykknes, Annette (main superv.) Kvittingen, Lise
Weggeberg, Hanne	Metal characterization of different size fractions of airborne particulate matter and adverse health effects in humans	Flaten, Trond P. (main superv.) Hilt, Bjørn
Wilhelmsen, Øivind	Non-equilibrium thermodynamics of phase transitions	Kjelstrup, Signe (main superv.)
Waage, Magnus	Kinetic properties of gas hydrates	Kjelstrup, Signe (main superv.) van Erp, Titus

MSc in Chemistry

Husby, Ingrid Supervisor: Examiners:	Sporelementer i drikkevann i Nord-Trøndelag Professor Trond Peder Flaten Dr. Bjørn Frengstad Professor Øyvind Mikkelsen
Jacobsen, Trygve Dragsloth Supervisor: Examiners:	SAPO-34 with Copper: Investigation of hierarchical pore characteristics and interactions with copper for catalytic applications Associate Professor Karina Mathisen Dr. Camilla Nordhei Associate Professor Hilde Lea Lein
Kirkmo, Fredrik Motland Supervisor: Examiners	Adam Lonicer's Kreuterbuch and 16th century distillation Professor Lise Kvittingen Associate Professor Olav Bjørlo Associate Professor Rudolf Schmid
Linde, Henrik Supervisor: Examiners:	Stereoselektiv addisjon av kirale sulfinimin til pyrrolderivat Associate Professor Odd Reidar Gautun Research Manager, dr. Scient. Hailing Liu Associate Professor Elisabeth E. Jacobsen
Ofstad, Benedicte Supervisors: Examiner:	Vibrational motion in molecules Professor Per-Olof Åstrand Kenneth Ruud Magnus Ringholm Dr. Heike Flieg
Pettersen, Iselin Esp Supervisors: Examiners:	Metallbelastning i Mo i Rana studert ved transplanterte moseprøver Professor Trond Peder Flaten Professor Emeritus Eiliv Steinnes Researcher Tor Erik Finne, NGU Professor Torunn Berg
Strand, Robin Viktor Supervisors: Examiners:	Characterization of ion selective membranes for application in reverse eletrodialysis systems Professor Signe Kjelstrup Odne Burheim Katrine Sandbakk Senior Researcher Torleif Holt Professor Øyvind Mikkelsen
Sylte, Kent Ove Kragseth Supervisors: Examiners:	Syntese av nye kinase antagonister med potensielt forbedrende medikamentelle egenskaper Associate Professor Bård H. Hoff PhD-candidate Steffen Bugge Research Manager, dr. Scient, Hailing Liu Associate Professor Nebojsa Simic
Vebøstad, Marie Tveit Supervisor: Examiners:	Undersøkelse av forurensning i jord i områder benyttet for brenning av sankthansbål Professor Øyvind Mikkelsen Professor Emeritus Knut Schrøder Professor Torunn Berg

MSc in Chemistry/Technology

Hauge, Hans Henrik R. Supervisors: Examiner:	Calorimetry and Exergy Analysis in the Context of Renewable Energy Devices Professor Signe Kjelstrup Associate Professor Odne S. Burheim, HiST Dr. Ing./Senior Researcher Preben Vie
Holden, Mia Cathrine Hellansjø Supervisors: Examiner:	Utvikling av Prosedyre for Overvåkning av Nickel og Kobolt i Avløpsvann fra Metallurgisk Industri Professor Øyvind Mikkelsen Researcher Torkild Eivindson Professor Emeritus Knut Schrøder
Moen, Ingrid Ullestad Supervisor: Examiner:	Fragment Based Approach in the Search for New Kinase Inhibitors Associate Professor Bård H. Hoff Associate Professor Anders Vik, UiO
Skjelbred, Kristin Marie Supervisor: Examiner:	Calculation of Transition Moments Using the Extended Coupled Cluster Model ECC2 Professor Henrik Koch Associate Professor Thomas Bondo Pedersen, UiO

MSc in Environmental toxicology and chemistry (MSENVITOX)

Vike, Kristine Supervisors: Examiner:	Oil Spill Forensics Professor Øyvind Mikkelsen Professor II Per Johan Brandvik Professor Emeritus Knut Schrøder
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MSc in Education, chemistry

Baardsgaard, Margrete Marine Supervisor: Examiners:	Innhold i kjemifaget Associate Professor Annette Lykknes Cand. Real. Brit Skaugrud Professor Lise Kvittingen
Børset, Kristine Supervisor: Examiner:	Uttesting av stabiliteten til DGT-prøvetakere for metallbestemmelse Professor Øyvind Mikkelsen Professor Emeritus Knut Schrøder
Børset, May Supervisor: Examiner:	Bruk av sporelementer som en indikator på potensielle endringer i kystvann, som følge av fiskeoppdrett Associate Professor Murat van Ardelan Professor Emeritus Jon-Arne Sneli
Damhaug, Marit Elisabeth Fors Supervisors: Examiners:	Studie av kvikksølv, svovel og naturlig organisk materialer i jord i Ny-Ålesund, Svalbard Professor Øyvind Mikkelsen Professor Emeritus Eiliv Steinnes Professor Torunn Berg Researcher Katrine Aspomo Pfaffhuber, NILU
Ekeland, Mari Helen P. Supervisor: Examiner:	Studier av elveosser og elveutløp i større elver i Trondheimsfjorden Professor Øyvind Mikkelsen Professor Emeritus Knut Schrøder
Eliassen, Sigve Supervisor: Examiners:	Kjemo-enzymatisk syntese av enantiomert rene halogenerte syklopropaner og triflatestere Associate Professor Elisabeth E. Jacobsen Associate Professor Anders Vik, UiO
Gjendemsjø, Eirin Supervisor: Examiner:	Miljøkartlegging av strøsand fra like geografiske lokaliteter i Trondheim, samt utlekkingsstudier av tungmetaller i forbindelse med gjenbruk Professor Øyvind Mikkelsen Professor Emeritus Knut Schrøder
Hald, Sara Jenny Katrine Supervisors: Examiner:	Kartlegging og studie av metaller og naturlig organisk materialer i elver på Svalbard Professor Øyvind Mikkelsen Professor Torunn Berg Professor Emeritus Eiliv Steinnes Researcher Katrine Aspomo Pfaffhuber, NILU
Hosking, Tone Supervisors: Examiner:	Utvikling av passiv prøvetakingsteknologi for miljøovervåking av metaller i det urbane vannsystemet Professor Øyvind Mikkelsen Associate Professor Tone Muthanna, IVM Researcher Øyvind Garmo, NIVA Professor Emeritus Knut Schrøder
Jenssen, Ida Helena Supervisor: Examiner:	Studier av elveosser og elveutløp i større elver i Trondheimsfjorden Professor Øyvind Mikkelsen Professor Emeritus Knut Schrøder
Kirkemo, Solvor Motland Supervisor: Examiner:	Kartlegging og studie av forurensning av avrenningsvann fra snødeponier i Trondheim til lokale bekker Professor Øyvind Mikkelsen Professor Emeritus Knut Schrøder
Nygard, Ingeborg Supervisors: Examiner:	Geokjemisk kartlegging av metaller i jord i Hamar by Professor Trond Peder Flaten Professor II Rolf Tore Ottesen Researcher Tor Erik Finne, NGU
Roset, Marianne Supervisors: Examiner:	Kartlegging og studie av forurensning av avrenningsvann fra snødeponier i Trondheim til lokale bekker Professor Øyvind Mikkelsen Senior Engineer Silje Salomonsen, Trondheim Kommune Professor Emeritus Knut Schrøder

PhD in Chemistry, finished 2014:

Bøyesen, Katrine Lie	Reactivity and Synergism of Vanadium in Microporous Supports with Copper as a Co-cation
Trial lecture	Methanol synthesis: state-of-art and future directions
Main supervisor	Associate Professor Karina Mathisen
Assessment Committee	Dr. Andrew Beale, University College London, Department of Chemistry, UK Dr. David Waller, Yara International ASA Associate Professor Bård Helge Hoff, Department of Chemistry, NTNU
Gerontas, Apostolos	Reforming separation: chromatography from liquid to gas to high performance liquid
Trial lecture	The significance of the instrumental revolution for the development of chemistry
Main supervisor	Associate Professor Annette Lykknes
Co-supervisor	Professor Klaus Hentschel
Assessment Committee	Professor Klaus Ruthenberg, Coburg University of Applied Sciences and Arts Professor Anders Lundgren, Uppsala University Professor Vassilia Partali, Department of Chemistry, NTNU
Karlsen, Morten	Synthesis of 13C-labeled drugs of abuse as internal standards for reducing differences in ion suppressing/alteration effects in LC/MS-MS quantification
Trial lecture	Chemical sensors for forensic purposes
Main supervisor	Professor Bård Helge Hoff, Department of chemistry, NTNU
Co-supervisor	Research manager Hailing Liu, Chiron AS
Assessment Committee	Associate Professor Robert Kronstrand, Linköping University, Sweden Professor Tore Lejon, UiT – The Arctic University of Norway Professor Anne Fiksdahl, Department of Chemistry, NTNU
Kaspersen, Svein Jacob	Synthesis and evaluation of pyrrolo-, thieno- and furopyrimidines as epidermal growth factor receptor tyrosine kinase inhibitors
Trial lecture	Multicomponent reactions in medicinal chemistry
Main supervisor	Associate Professor Bård Helge Hoff, Department of chemistry, NTNU
Co-supervisor	Associate Professor Eirik Sundby, Sør-Trøndelag University College
Assessment Committee	Professor Morten Grøtli, Institutt for kemi og molekylärbologi, Göteborgs Universitet Professor Lise Lotte Gundersen, Kjemisk institutt, Universitetet i Oslo Associate Professor Odd Reidar Gautun, Department of Chemistry, NTNU
Saepurahman	Infrared spectroscopic studies of zeotype and zeolite catalysed hydrocarbon/oxygenate conversion reactions
Trial lecture	Heterogenous catalysis studied by operando spectroscopy
Main supervisor	Associate Professor Karina Mathisen, Department of Chemistry, NTNU
Co-supervisor	Associate Professor Stian Svelle, Department of Chemistry, Univ. of Oslo
Assessment Committee	Dr. Justin Hargreaves, Department of Chemistry, University of Glasgow Dr. Knut Thorshaug, SINTEF Materialer og Kjemi Associate Professor Nebojsa Simic, Department of Chemistry, NTNU
Skorpa, Ragnhild	Hydrogen dissociation under equilibrium and non-equilibrium conditions
Trial lecture	Strengths and limitations of classical potential models for gas-phase chemical reactions and their use in computer simulations
Main supervisor	Professor Signe Kjelstrup, Department of Chemistry, NTNU
Co-supervisor	Professor Emeritus Dick Bedeaux, Department of Chemistry, NTNU
Assessment Committee	Prof. Dr. Nico van der Vegt, Technical University of Darmstadt, Germany Research Scientist Stefan Anderson, SINTEF Materials and Chemistry, Norway Professor Bjørn Hafskjold, Department of Chemistry, NTNU

PhD in Chemistry, continued:

Voldsund, Mari

Trial lecture

Main supervisor

Co-supervisor

Assessment Committee

Exergy analysis of offshore oil and gas processing

What can exergy analysis bring to renewable energy providers?

Professor Signe Kjelstrup, Department of Chemistry, NTNU

Professor Ivar Ståle Ertesvåg, Department of Energy and Process Engineering, NTNU

Prof. Dr. Ir. Jo Dewulf, Ghent University, Belgium

Dr. Tore Myhrvold, Det Norske Veritas

Professor Bjørn Hafskjold, Department of Chemistry, NTNU

Zaidi, Asma

Trial lecture

Main supervisor

Co-supervisor

Assessment Committee

Polyenoic acids and their alkali and europium salts: Synthesis. Surface Properties. Antioxidant properties

Rare Earth elements - applications in physics, chemistry and medicine

Professor Vassilia Partali, Department of Chemistry, NTNU

Hans-Rickard Sliwka, NTNU

Professor Bernd Schäfer, Universität Heidelberg, Germany

Professor Yaser Ahamad Yousef, Chemistry Department,

Yarmouk University, Jordan

Associate Professor Nebojsa Simic, Department of Chemistry, NTNU



Iceshelf, Antarctica ©M.Ardelan

Post Graduate Students

Student exchange to NTNU, Department of Chemistry

Name	Institution
Belkhodja, Yacine	Université Paul Sabatier, Toulouse, France
Boniolo, Manuel	Università degli Studi di Padova, Italy
De Clerck, Jonathan L.	Katholieke Universiteit, Leuven, Belgium
Demaret, Lucas	Université de Liège, Belgium
Devos, Julien André	Katholieke Universiteit, Leuven, Belgium
El Assimi, Aimen	Université Paris Descartes, France
Escude Font, Joel	Universitat Politècnica de Catalunya, Spain
Ghesquiere, Charles Pieter	Katholieke Universiteit, Leuven, Belgium
Gmelch, Tobias Johann	Technische Universität München, Germany
Gossele, Ans Helena	Katholieke Universiteit, Leuven, Belgium
Novillo Sanjuan, Olga	Universitat de València, Spain
Renaudin, Lea Nadine S.	Institut national des Sciences appliquées de Rouen, France
Schmidt, Jeppe Lunde	Danmarks Tekniske Universitet, Denmark
Syrjänen, Anna Sophie	Åbo Akademi, Finland
Vareka, Martin	Vysoká škola chemiko-technologická Praze, Czech Republic
Vendredy, Leen	Katholieke Universiteit, Leuven, Belgium
Vranken, Thomas	Katholieke Universiteit, Leuven, Belgium

Student Exchange from NTNU, Department of Chemistry

Name	Specialization	Level	Institution
Aae, Bjørn Erik	MTKJ-Org.chem	MSc, 4th yr	TUM, Germany
Ali, Daniel	MKJ-Struc. chem	MSc, 4th yr	University of Newcastle, Austr.
Evjen, Sigvart	MTKJ-Org.chem	MSc, 4th yr	RWTH Aachen, Germany
Haarseth, Pia	MTKJ-Org.chem	MSc, 4th yr	University of Western Australia
Lindberg, Daniel	MTKJ-Org.chem	MSc, 4th yr	TUM, Germany
Leraand, Camilla Mosbakk	BKJ- Org.chem	BSc, 3rd yr	University of Buenos Aires, Arg.

Scientific Staff

Organic chemistry



Group Leader
Associate Professor, Dr.ing.
Odd Reidar Gautun



Professor, Dr.ing.
Anne Fiksdahl



Professor, Dr.rer.nat.
Vassilia Partali



Associate Professor,
Dr.Scient
Bård Helge Hoff



Associate Professor, Dr.Scient.
Elisabeth Egholm Jacobsen



Associate Professor, Ph.D.
Nebojsa Simic

Staff

Applied Theoretical Chemistry



Group Leader
Professor, Dr.scient.
Bjørn Kåre Alsberg



Associate Professor, PhD
Titus Sebastiaan van Erp



Professor, Dr.techn.
Signe Kjelstrup



Adjunct Professor
Fernando Bresme



Professor , Dr.techn.
Bjørn Hafskjold



Professor, Ph.D.
Henrik Koch



Associate Professor, Ph.D.
Ida-Marie Høyvik



Professor, Ph.D.
Per-Olof Åstrand

Environmental and Analytical Chemistry



Group Leader
Associate Professor, Dr.rer.nat.
Rudolf Schmid



Adjunct professor
Per Johan Brandvik



Associate Professor, Ph.D.
Karina Mathisen



Associate Professor, Dr.Scient
Murat V. Ardelan



Professor, Dr.ing.
Trond Peder Flaten



Professor, Dr.Scient
Øyvind Mikkelsen



Associate Professor, Dr.ing.
Florinel G. Banica



Professor, Dr.Scient.
Lise Kvittingen



Professor, Ph.D.
David Nicholson



Professor, Dr.scient.
Torunn Berg



Adjunct Professor
Rolf Tore Ottesen

Staff

Administrative staff



Head of department
Marie-Laure Olivier



Higher Executive Office
Gerd Flataas



Higher executive officer
Bjørn Syvertsen



Executive officer
Thea Berg Fines



Executive officer
Eva Madland



Higher executive officer
Ingrid Kristine Tømmerdal



Administrative manager
Gunhild Meistad

Technical staff



Technical manager
JonErik Aaseng



Head engineer
Susana Villa Gonzalez



Staff engineer
Marit Syversveen



Staff engineer
Stein Almo



Head engineer
Nina Klausen



Staff engineer
Gunnar Svare



Staff engineer
Julie Asmussen



Head engineer
Syverin Lierhagen



Staff engineer
Roger Aarvik



Head engineer
Anica Simic

Staff

Emeriti at Dept. of Chemistry

Thorleif Anthonson
Jan Bakke
Terje Bruvoll
Dick Bedeaux
Kolbjørn Hagen
Synnøve Liaaen Jensen
Knut Schrøder
Eiliv Steinnes
Reidar Stølevik

Student assistants

Spring 2014

Barsnes, Anne
Bekkevard, Pål Unnerud
Brondz, Anton Christian
Eraker, Øyvind Juvkam
Eriksen, Nora Meling
Folkestad, Sarai Dery
Galteland, Olav
Kjønstad, Eirik
Kringhaug, Henrik Holthe
Lauvås, Anna Jacobsen
Lea, Kristoffer Larsen
Leithaug, Trygve
Lindland, Kim
Moen, Ingri Ullestad
Nervik, Sondre
Nguyen, Anh Quynh Ngoc
Nøkleby, Christina
Prytz, Halvor
Reiersølmoen, Ann Christin
Ringvold, Anna
Sylte, Kent-Ove Kragseth
Thorstensen, Eivind Bruun
Willumsen, Fredrik

Scientific assistants

Magnus Heskestad Waage
Emilio Catelli
Daniel Lisø
Tina Kristiansen
Ragnhild Beate Strand Østrem
Jon Erik Aaseng
Marit Syversveen
Henrik Linde
Anica Simic
Thomas Aleksander Bakka
Fredrik Willumsen
Eirik Hjertenæs
Mehdi Mahmoodinia
Kristin Marie Skjelbred
Julie Asmussen
Nina Brochs Klausen
Rajesh Raju
Asma Zaidi
Eva Madland
Susana Villa Gonzalez
Nazanin Davari

Student assistants

Fall 2014

Aarøen, Ola
Adnan, Mohammed Mostafa
Amundsen, Filip
Brondz, Anton Christian
Bruvold, Are Sæle
Buene, Audun Formo
Elvheim, Andrea Iselin
Engstrøm, Mia
Eriksen, Nora Meling
Evenstad, Otto Magnus
Falck, Merete
Fauskanger, Tine Olsen
Flo, Jørgen
Folkestad, Sarai Dery
Galteland, Olav
Grorud, Bettina
Grønvold, Julie
Haslund, Vilde Stubberud
Jørgensen, Ingrid Kvinge
Kjønstad, Eirik
Lauritsen, Christian
Lea, Kristoffer Larsen
Leirvåg, Ida
Leithaug, Trygve
Lien, Størk
Lund, Marlene Louise
Lundgren, Mathias Kristoffer
Ottestad, Anine Larsen
Reiersølmoen, Ann Christin
Ringvold, Anna
Solberg, Amalie
Stakvik, Linda
Stubhaug, Mia
Thorfinnsdottir, Lilja Brekke
Torp, Eirik
Ueland, Åsmund Stenhaug
von Blokland, Irene Vera
Walderhaug, Martin
Yeboah, Isaac

Guest professors/researchers/lecturers

Kate McAulay, guest researcher	31.10.2014 – 14.11.2014
Marta Marty (Spania) guest researcher	3.7.2014 – 31.10.2014
María del Camino Martín Torre, guest	2.7.2014 – 31.10.2014
Ana Rocio Borrero Santiago, guest	2.7.2014 – 31.10.2014
So Hyun Kwak, guest	2.9.2014 – 30.9.2014
Anna Zhyrova, guest	6.3.2014 – 5.5.2014 5.11.2014 – 31.12.2014
Dr.rer.nat. Richard Sliwka, guest researcher	1.1.2014 – 31.12.2014
Dr. Kang Xue, guest researcher, Faculty of Resources and Materials, Northeastern University at Qinhuangdao, China.	26.6.2013 – 30.4.2015
Professor Ketil Hylland, Department of Biosciences, University of Oslo, guest lecture: "Offshore oil and gas production - Environmental consequences"	16.10.2014
Associate Professor Mark Hermanson, University Centre in Svalbard (UNIS), guest lecture: "Organic contaminants on Svalbard: What are they? How much is there? What are the likely sources? Results from research in the abiotic world at UNIS."	9.10.2014
Heike Fliegl, University of Oslo. What are magnetically induced current densities good for?	12.8.2014
Magnus Ringholm, University of Tromsø, Analytical molecular properties with OpenRSP: applications in vibrational spectroscopy.	12.8.2014
Prof. Dr. Nico van der Vegt, Computational Physical Chemistry Center of Smart Interfaces, Technical University of Darmstadt, Germany. Challenges in multiscale simulations of soft matter.	26.11.2014
Dr. Santiago Cuesta-Lopez, Advanced Materials, Nuclear Technology, Applied Nanotechnology, University of Burgos. Spain. Multiscale Modelling and genome materials initiative: metals and alloys in extreme environments.	21.5.2014
Dr. Uli Aschauer, Materials Theory, ETH Zürich, Switzerland. Structure, defects and reactivity of transition metal oxide surfaces.	21.5.2014
Dalibor Stys, Prof., deputy director Institute of complex systems, University of South Bohemia, Nové Hradý, Czech Republic.	26.11.2014
Yoriko Atomi, phd, Project Professor, Faculty and Graduate School of Engineering, Tokyo University of Agriculture and Technology, Japan. Connection of cell and body layers through dynamics/spontaneity/emergence and adaptation/ learning.	11.9.2014

Annual Report for Department of Chemistry 2014



NTNU – Innovation and Creativity

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

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