



Faculty of Natural Sciences
and Technology
Department of Chemistry

Master's thesis proposals

Department of Chemistry

Academic year 2017-2018

This document contains master's thesis proposals for the following programmes of study:

Master in Chemistry (MSCHEM)
All specializations

Master in Environmental Toxicology and Chemistry (MSENVITOX)
Specialization: Environmental Chemistry

Master in Chemical Engineering and Biotechnology (MTKJ and MIKJ)
Main profile: Chemistry

Natural Science with Teacher Education (MLREAL)
Main subject: Chemistry

Please contact the supervisor directly if you have any questions related to the proposed projects.

Master Thesis in Organic Chemistry, Department of Chemistry

Synthesis and characterization of organic dyes for dye-sensitised solar cells



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Project title: **Proving the stereochemistry of dyes by NMR spectroscopy**

Phenothiazines containing a terminal cyanoacrylic acid, such as compound 3, are suitable dyes for dye-sensitised solar cells (DSSC). The cyanoacrylic acid moiety is essential since it binds to the titanium dioxide and ensures an efficient injection of electrons from the excited dye to the TiO_2 , see Figure 1.

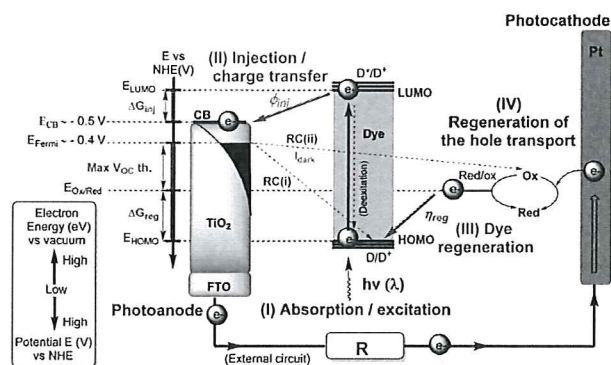


Figure 1. Energetic diagram of an operative and conventional (n-type) TiO_2 -DSSC using a redox couple in the electrolyte

Whereas, it is generally assumed that the carboxylic acid is trans to the aromatic system, this has seldom been proved. The groups of Hoff and Gautun are working with phenothiazine dyes, and a number of derivatives are available for studies. Model structures are also easily synthesised from intermediate precursor by the well-known Knoevenagel reaction. Initial studies indicate that only one isomer is formed. However, the stereochemistry has not been proved. It can be assumed that proof of the stereoselectivity can be achieved by the measurement of the coupling constants $^3J(^1\text{H},^{13}\text{C})$ of the olefinic hydrogen atom with the COOH and CN groups or by the heteronuclear Overhauser effects (HNO) between these substituents and the olefinic hydrogen. Possibly, the synthesis of carbon 13-labelled derivatives would ease this assignment.

There is place for 1 master student on this project.

Biocatalysis in organic chemistry

Synthesis of enantiopure bioactive molecules by use of biocatalysts



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Project suggestions

Chemo-enzymatic synthesis of enantiopure drugs and other bioactive compounds

Many drugs are secondary alcohols with a terminal amino group. Many of these drugs are manufactured with active pharmaceutical ingredients (API) in the racemic form, a few are manufactured as a single enantiomer. However, single enantiomer drugs are preferred due to possible side effects of the "wrong" or less active enantiomer. In drug synthesis use of enzymes as lipases, reductases and other enzyme classes as chiral catalysts may give up to 99% enantiomeric purity (ee), and the processes are regarded as "green chemistry" due to mild reaction conditions and re-use of the catalyst many times. Examples of chemo-enzymatic synthesis of enantiopure compounds by us are listed below [1-3]. Development of enzyme catalysed methods for synthesis of pure enantiomers involves synthesis of racemic compounds, enzyme catalysed kinetic resolutions or direct asymmetrisations, analyses of enantiomers on chiral GLC and HPLC-columns, and finally use of the enantiopure building blocks in synthesis of the drug. (30 or 60 ECTS). Alprenolol, sotalol and metipranolol are interesting targets, see fig. 1. When we synthesise single enantiomer drugs, many questions arise about the processes and enzyme mechanisms [4]. For 60 ECT master projects these topics may be interesting, and project descriptions will be outlined in accordance with the ongoing activity in the group.

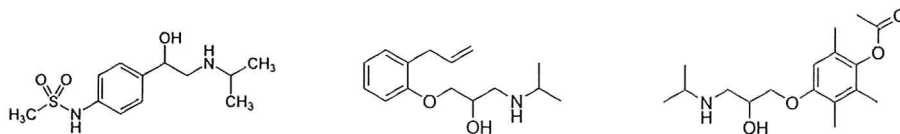


Figure 1. From left to right: Sotalol, alprenolol and metipranolol.

References

1. *Enantiopure dihalocyclopropyl alcohols and esters by lipase catalyzed kinetic resolution. J. of Biotechnol.* **2013**, *168*, 284-288.
2. *2-C-Methyl-D-erythritol. Produced in plants, forms aerosols in the atmosphere. A new pathway to isoprenoids. Biocatalysis & Biotransformation*, **2015**, *33(4)*, 191-196
3. *Highly enantioselective CALB-catalyzed kinetic resolution of building blocks for β -blocker atenolol, Tetrahedron*, **2016**, *72*, 7288- 7292, 10.1016/j.tet.2016.02.018
4. *Desymmetrization of cbz-serinol catalyzed by crude pig pancreatic lipase reveals action of lipases with opposite enantioselectivity, J. Mol. Catal. B* **2013**, *85-86*, 134-139

Environmental and analytical chemistry

Research fields: Trace elements in the environment and human health



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Project suggestions

Most of these projects can be adjusted to fit to a 30 or 60 ECTS credit assignment (if there is a specific number of credits, remember to mark the assignment)

1. Mapping of the contents of trace elements / heavy metals in various foodstuffs, drinks, foods, etc. (input from the student!), focusing on health implications. Previous master projects in this field include drinking water, tea, dietary supplements and baby food.
2. At our department, we have a large collection of samples of vegetation, soil and other material representing the whole country or specific geographical regions. These samples were collected to gain knowledge of both the natural distribution of trace elements and the influence of regional and local pollution. However, at the time of collection we did not have access to the high-quality analytical instruments that we now have, so it would be very interesting to analyse these valuable samples using ICP-MS. Master projects using some of this material could be supplemented by collecting additional samples in the field (e.g. to investigate possible time trends).
3. Projects in cooperation with the Environmental unit in Trondheim municipality (Miljøenheten i Trondheim kommune), on streams and lakes around Trondheim, air quality, harbour sediments (Prosjekt "renere havn" (www.renerehavn.no)), etc.

Applied Theoretical Chemistry

Molecular Modeling

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Project suggestions

These projects can be adjusted to fit to a 30 or 60 ECTS credit assignment. The project descriptions more describe a theme/research area of interest rather than one specific M.Sc. project. The individual project will be defined together with the student.

1. Electrical insulation in liquids

We have a long-term collaboration with SINTEF Energy and ABB Corporate Research in Västerås, Sweden to understand electrical breakdown in liquids at an atomistic level. A project would normally involve quantum chemical calculations of ionization and/or electron attachment processes in high electric fields. At the moment, we are also interested in calculating cross-sections (i.e. probabilities) for processes related to electron-molecule collisions and photoionization. Additional work includes the calculation of chemical reaction barriers for the dissociation of hydrocarbons in high electrical fields and the kinetics of such processes using kinetic Monte Carlo simulations.

2. Catalysis: metal particle - molecule interactions

In several research fields, it is of high interest to accurately model interactions between molecules and metal particles, and for this purpose we use density-functional theory (DFT) calculations. In collaboration with Prof. De Chen in the Catalysis group at NTNU, we study e.g. Pt and Co clusters on carbon support materials like graphene and how the interactions with the carbon material affect the catalytic activity of the metal atoms. In addition, we study molecule-coated nanoparticles, e.g. gold particles, which are important for applications in optics (with Fernando Bresme, Imperial College London).

3. Classical polarization models

We work on establishing "classical" models for electronic polarization and electron transport processes based on classical electromagnetism and concepts from force fields as well as relating these models to quantum mechanics. This type of projects is more "theory-oriented" and may involve both mathematical derivations as well as software development in addition to calculations. Optical properties that we are currently interested in includes second-harmonic generation spectroscopy at interfaces (also with F. Bresme). A project may also be carried out in collaboration with the group at the University of Copenhagen that has an expertise in "molecular electronics".

Quantum Chemistry

Development and application of electronic-structure methodologies

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Project suggestions

Most of these projects can be adjusted to fit to a 15, 30 or 60 ECTS credit assignment. Project 1 is suitable for a student who is interested in exploring the quantum chemical nature of molecular without doing theoretical developments, while projects 2-4 are suitable for students who are interested in theoretical developments and /or computer programming.

1. Calculations of molecular properties
Molecular properties such as geometries, excitation energies, responses to magnetic and electric fields etc. can be accurately determined using quantum chemical methods. In this project, existing methods will be used to explore the properties of a molecule of interest.
2. Multi-level coupled cluster theory development
Coupled-cluster theory is a highly successful hierarchy of wave function models to accurately describe molecular systems. However, its computational cost limits its use to rather small systems. The multi-level coupled-cluster model, developed at NTNU, exploits the locality of electronic properties to make coupled-cluster calculations more efficient. In this project, you will participate in current theoretical developments in multi-level coupled cluster.
3. Extending the applicability range of Hartree-Fock theory
Hartree-Fock theory is the cornerstone for accurate ab-initio electronic-structure theories, and in itself Hartree-Fock gives a decent approximation to energies and molecular properties for molecular systems dominated by a single electronic configuration. The Hartree-Fock wave function can be applied to relatively large systems, but it is of interest to extend the applicability range even further, so that it may be applied to e.g., molecules in solutions or for active sites of enzymes.
4. Hartree-Fock theory in a non-orthogonal molecular orbital basis
In developments of low-scaling correlated wave function models, most methods relies on the spatial locality of the molecular orbitals employed. Spatial locality of orbitals is improved when relaxing the orthogonality constraint and it is therefore of interest to develop a non-orthogonal Hartree-Fock framework, to explore the possibilities offered by the non-orthogonality of the orbitals.
5. Other applications or theoretical developments projects may also be created. Send an email or come talk to us.

Synthetic Organic chemistry

Gold(I) catalysis in organic synthetic chemistry (<https://www.ntnu.edu/gold>)



Professor Anne Fiksdahl

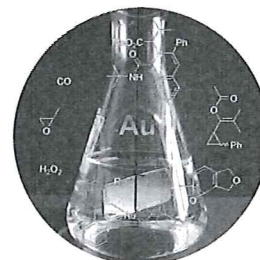
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Master Projects

The main objectives of the project are:

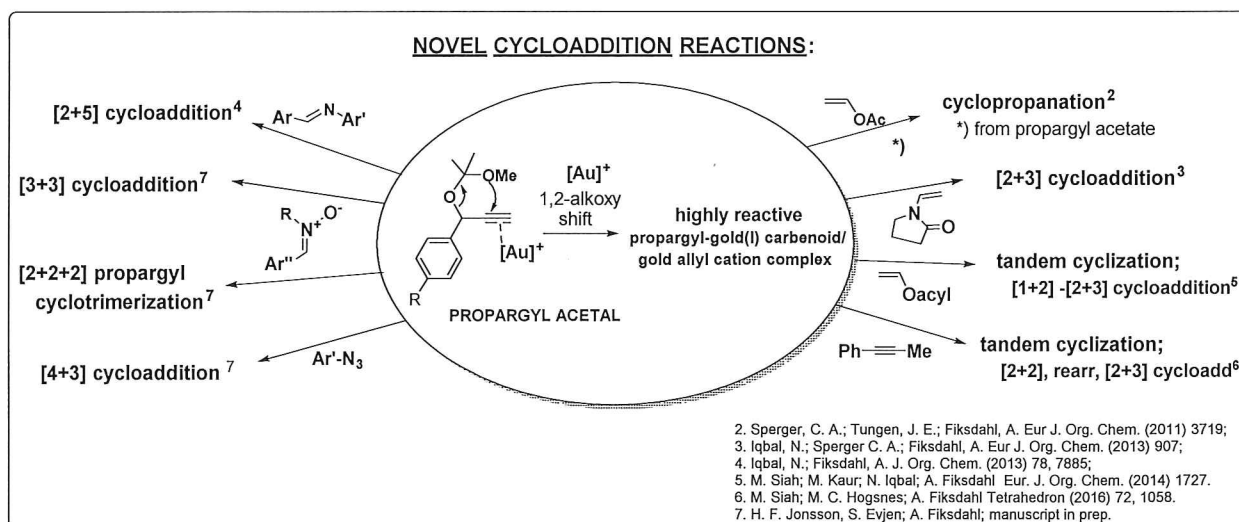
- develop **new selective gold catalysed cyclization reactions**,
- incl **mechanistic** studies (e.g. isotope labelling, NMR spectroscopy)
- **elucidate structure** of novel compounds.

Projects (30/60 ECTS credits) on current research topics in the group will be defined by contact with prof. Anne Fiksdahl

Background gold catalysis in the Fiksdahl group

Gold(I) catalysis of organic reactions has become a rapidly expanding field in recent years after being neglected by organic chemists for a long time. Gold(I) catalysts react in very selective ways and may give access to highly complex molecules and challenging new structures. Alkynes are successfully used as substrates for gold catalysis.

The Fiksdahl group is working with advanced metal-organic catalysis in organic synthesis. We have shown that specific highly reactive and versatile substrates are able to follow a diverse range of novel Au(I)-catalysed chemoselective pathways, as shown by published results from current and previous master / PhD projects in the group. The novel approaches readily allow preparation of a great variety of new complex poly-functionalised products:



Synthetic Organic chemistry

Synthesis of novel absorbents with optimal CO₂ capturing properties



Professor Anne Fiksdahl

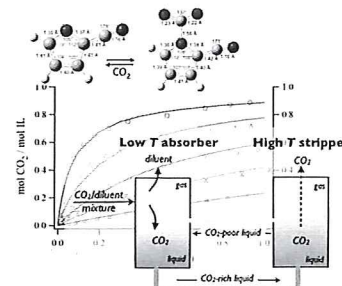
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Master Project

The main objectives of the project are:

- synthesize new promising absorbents (amines, imidazoles, ionic liquids/ILs) for CO₂ capture, based on theoretical calculations;
- characterize and test newly synthesized absorbent candidates (thermodynamic and solvation properties)

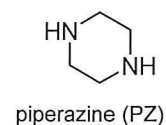
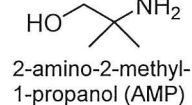
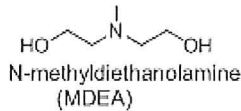
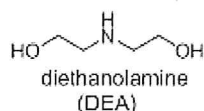
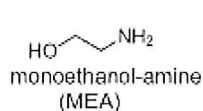
in order to obtain adsorbents with optimal reactivity toward CO₂, and greatly reduced absorbent regeneration energy, without sacrificing environmental friendliness and operational stability. The project will involve classical organic synthetic chemistry (incl. purification, characterization; flash chrom. recryst., dest, ion exchange, NMR, IR, HRMS).

Projects (30/60 ECTS credits) will be defined by contact with prof. Anne Fiksdahl.

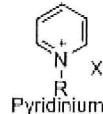
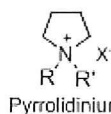
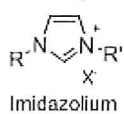
Background CO₂ capture:

Capturing CO₂ using absorption with amine solutions has been used industrially for years:

a) Organic amines (*prim/sec/tert*) being used for CO₂ capture:



b) Structures of ILS:



In order to meet the goals for global reduction of CO₂, an improvement of current technologies for carbon dioxide capture and storage (CCS) is needed. Hence, the efficiency of new methods and their suitability for large-scale industrial applications must be increased.

- *The present project* is applying *de novo* design to develop improved new absorbents.
- The most promising candidates for CO₂ capture absorbents is prepared by org. synthesis.
- A microscale measurement equipment is built at SINTEF Matr. and Chem. as part of the project in order to enable experimental testing of small amounts of synthesized absorbent.
- Accurate measurements of the most important thermodynamic properties give information on the CO₂ absorption capacity.

The present project is aiming at increasing the efficiency of amine-based capture technology to be applied in the development of the next generation of absorbents, such as new amines, imidazoles and ionic liquids (ILs, see b) above).

The Fiksdahl group is responsible for the organic synthesis and testing part of the project.

Chemometrics and Chemoinformatics

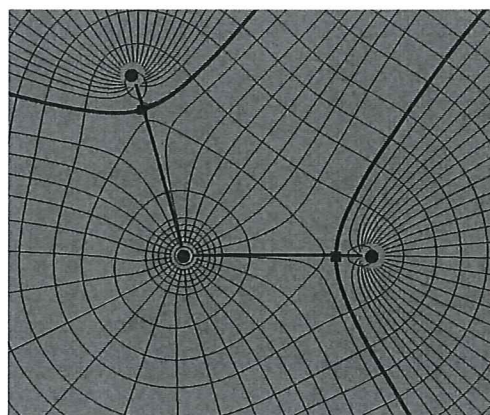
Applications to new materials for organic solar cells



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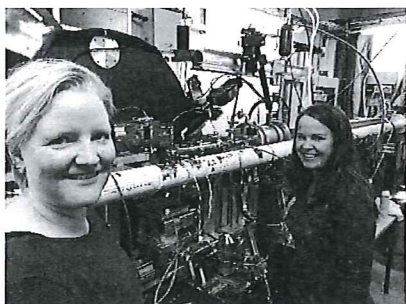
Master project suggestions. The master projects done in our group will be linked to ongoing research in the field of organic solar cells. There is a need to develop methods for cheaper and more efficient development of photovoltaic materials, in particular organic solar cell materials. We use a fragment-based evolutionary *de novo* design approach to propose new compounds with improved photovoltaic properties. In particular we study dye molecules in dye-sensitized solar cells (DSSC).

1. ***de novo* design of new solar cell dyes with optimal properties using principal properties.** A drawback with evolutionary *de novo* methods is that they require a large amount of computer resources. Another, approach is to employ *principal properties (PP)* in combination with experimental design. Each fragment is described by a set of scores which have been derived from a principal component decomposition of a matrix containing multiple fragments with variables describing their molecular structure.
2. **Building quantitative structure-property relationships (QSPR) models of solar cell dyes using Atoms in Molecules (AIM) electronic descriptors.** Forming predictive QSPR models for solar cell dyes requires descriptors that effectively capture the 3D electronic structure of molecules. Here descriptors based on bond critical points (BCPs) of the 3D electron density of molecules (from atoms in molecules (AIM) theory) will be investigated.
3. **Conformation dependent QSPR descriptors.** Many 3D structure descriptors are based on the geometry of the most stable conformation of a molecule. However, multiple conformations are important to understanding the properties of a molecule. Here, different approaches for incorporating conformational change in 3D descriptors is investigated.



Structural chemistry

Application of synchrotron techniques in material science and nanotechnology



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The research group consists of one post doc, two PhD's and currently 6 master students. A master project typically involves synthesis and functionalisation of new materials, such as metal containing aerogels or zeotypes. You will be trained in a range of characterization techniques such as XRD, BET, SEM, FTIR, all crucial for understanding the material. We travel frequently to synchrotrons like the ESRF in Grenoble to do x-ray absorption spectroscopy (XAS) to further study our materials at the Swiss Norwegian Beamline (SNBL). We have collaborations with University of Glasgow UK and Newcastle Australia.

Project suggestions

Most of these projects can be adjusted to fit to a 30 or 60 ECTS credit assignment.

1. Co-introduction of Co and Mo into mesoporous SBA-15 for the ammonia synthesis
2. Developing a synthesis route for functionalisation of silica aerogels with Re

Our ongoing collaboration with University of Glasgow investigating the effect of Re and Mo on cobalt-supported materials for the ammonia synthesis.

3. Functionalisation of Fe into silica aerogels; structural effect of metal loading

The goal is to develop single-site iron in hydrophobic aerogels which are interesting for a range of catalytic application.

4. Characterisation of hierarchical SAPO-34; are micro and mesopores available
5. Investigating the effect of porosity Cu-zeotypes for the reduction of NO_x

We are currently trying to make porous materials with super-highways for gas reactants travelling to micro reactors inside the material.

Master Thesis in Organic Chemistry, Department of Chemistry

Synthesis and characterization of bioactive compounds



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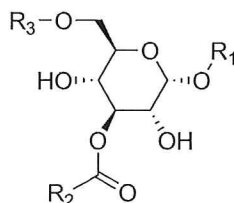
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Project title: Cancer treatment effects of selected intermediates in synthesis of unsaturated acyl glucoside.

***In vitro* experiments using photodynamic therapy (PDT) on cancer cell lines**

The work is mainly comprised of evaluation of anti-tumor activity of selected acyl glucosides synthesized in an ongoing research project at Dept. of Chemistry.



Laboratory work regarding sample preparation and purification will be performed at Dept. of Chemistry and cancer cell experiments (*in vitro*) at a suitable sterile cell laboratory. Various 1D and 2D NMR experiments, as well as HPLC and MS analyses, will be applied.

Methods: Actual technologies are Photodynamic therapy (PDT) and Photochemical Internalization (PCI) using isolated compounds in combination with disulfonated tetraphenyl chlorine isomers (TPCS_{2a}, Amphinex®), using a novel technology for targeted macromolecule delivery¹. The light treatment will be performed by suitable light sources in other research groups. Viability assays (MTT-experiments, clonogenicity) on different cancer cells after treatment by compounds of interest and light.

There is place for one master student on this project.

¹ Berg et al., Photochem Photobiol. Sci. 10, 1637-51 (2011).

Analytical Chemistry



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Project suggestions

Most of these projects can be adjusted to fit to a 30 or 60 ECTS credit assignment.

Master projects within;

- developing analytical methods and routines for industry and environmental monitoring.

Please contact me for detailed projects (e.g. specific projects connected to the aquaculture industry, metallurgical industry etc.)

Organic chemistry

Polyenes

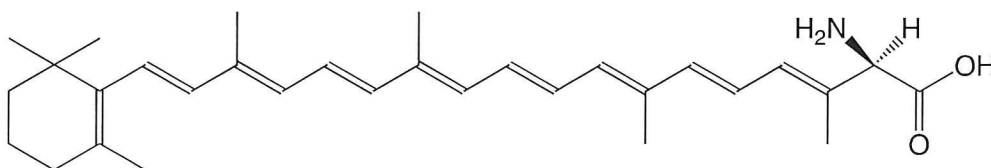


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Synthesis of highly conjugated unsaturated amino acids

Essential amino acids are saturated compounds. The few natural or synthetic mono or diunsaturated amino acids show distinct biological properties, e.g. as antibiotics and enzyme inhibitors. Highly unsaturated conjugated amino acids have not been detected in nature and have not been synthesized.

The aim of this master project is the synthesis of a highly unsaturated conjugated amino acid (1).



1

An obvious first try to polyene amino acids would be the classical Strecker reaction. Treatment of a polyunsaturated aldehyde with primary amines in the presence of molecular sieves could afford the corresponding imine, which, without isolation, would react with trimethylsilylcyanide (TMSCN) to nitrile. The hydrolysis reaction $-CN \rightarrow -COOH$ is expected to be the most demanding step in the reaction to unsaturated amino acid. The rather harsh reaction conditions have certainly to be modified to keep yields acceptable.

Alternatively, a polyene aldehyde or polyene ketone is treated with KCN, ammonium acetate or ammonium carbonate affording the corresponding hydantoin, which can be hydrolysed to the amino acid (Bucherer-Berg synthesis).

Another possible synthesis route is based on a Wittig reaction starting from a commercial amino acid, which after several transformations, (protection of amino group and reduction to alcohol, will react with the Wittig salt of a carotenoid.

Environmental Chemistry

Marine Organic Environmental Chemistry



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Project suggestions (can be adjusted to both 60 and 30 credits)

1. Oil spill forensics – Mapping sources for illegal oil spills

SINTEF is the national laboratory for oil spill identification in Norway. MSc projects are available focusing either on available data from the established database at SINTEF for fingerprinting and identification of possible sources for illegal oil spills. The information from an oil spill sample (gas chromatography and mass-spectrometry) is compared with the database by using both univariate statistics (t-test) and more sophisticated multivariate statistics. One focus on such a project could be to utilize more of the analytical data generated and study how oil weathering processes (e.g. evaporation, biodegradation and photo-oxidation) influence oil spill identification by using modern multivariate statistical methods. A large dataset of stranded oil spills are available from earlier KJ3050 field surveys along the coastline outside Trondheim. Also this year KJ3050 will perform a survey for new samples. These samples can be analyzed to determine the sources for these oil spills (offshore installations in the North Sea, coastal traffic (ships) or even foreign sources) Students could do their own analysis on new or stored oil samples or work on already generated data from earlier oil spills.

2. Fate of subsurface releases of oil (blow-outs) as a function of release conditions and oil types

The Macondo oil spill in the Mexico gulf in 2010 created new interest and focus on this special type of oil spills. This has been an important research field at SINTEF for the last twenty years. We perform both theoretical and experimental analytical projects regarding the physics, fate and modeling of subsurface oil releases. We have both basin and bench-scale experimental facilities we use in our projects. We study droplets size distributions of the released oil as a function of release conditions, oil chemistry and injection of surface active components (dispersants). Students can work on already generated data, participate in ongoing industry project at SINTEF or generate their own data with our bench-scale apparatus.

3. Weathering processes in marine oil spills

When oil is released or spilt in the marine environment many weathering processes will alter the chemical and physical properties of the oil as a function of time (emulsification, evaporation, photo-oxidation, natural dispersion etc.). Knowledge regarding how changes in these properties influence the properties of the oil spill is important for both understanding environmental damage and choice and effect of oil spill contingency methods.

Other MSc projects related to marine organic pollutants, initiated by students, could also be of interest. Do not hesitate to make contact for further discussions!

Molecular Modeling

Development of Advanced Simulation Techniques



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Project suggestions

In our group there are several possibilities for master projects. We welcome students from many study directions. Depending on personal interest, a master-thesis project can be pure theoretical (pen-and-paper mathematics), involve programming, or simply use existing software for running simulations and analyzing data. Contrary to what students often believe, one does not have to be a mathematical genius to perform a research project within theoretical chemistry. It is possible to go into depth regarding theory or software development if you want, but a lot of exciting research is done by applying existing programs in a similar way as an experimentalist uses an instrument. An interdisciplinary master-project is possible since we are dealing with many types of challenges, which could be tackled by chemists, mathematicians, computer scientists, chemical engineers, nanotechnology students, biotechnologists, or physicists. Here we list possible projects, though these are a few of the possible projects and if you have an own idea, I am happy to discuss it with you!

- 1. QUANTIS: a new way to combine classical dynamics and quantum-mechanics.**
In this master project you will contribute to our main research activity which implies a completely new way to combine classical molecular dynamics and quantum mechanics (See e.g. Nobelprize chemistry 2013) . The revolutionary new aspect that we are developing is that we connect these methods in the **time** domain not just in space. The method would allow us to study enzymatic and complex catalytic reactions involving large systems, long time-scales at quantum mechanical accuracy.
- 2. Coalescence and film rupture.** In this project reaction path sampling will be applied to study the film rupture between bubbles present in liquid emulsions, which is a key phenomena in coalescence process. The selected case of study consist in oil-water emulsions, which is a relevant system for oil industry.
- 3. Understanding DNA Dynamics.** For decades, experimental and theoretical scientists have been fascinated by the thermal DNA denaturation. It is biologically relevant since the opening of the double helix in an important step for the transcription of the genetic code. We have tested and developed simplified models to simulate the movements of DNA. In addition we developed special algorithms to run simulations much faster than was possible before. This allows us now to get a better idea on how the rate of denaturation changes with respect to the sequence and other factors. In addition, it allows us to test and compare results with experiments and to improve present models with this information.
- 4. MORE INFO ON THE WEBSITE: www.van-erp.org/**

Organic Analytical Chemistry



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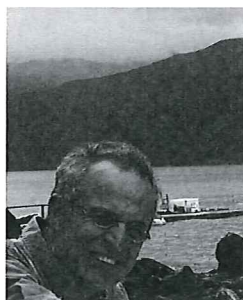
Project suggestions

Most of these projects can be adjusted to fit to a 30 or 60 ECTS credit assignment.

1. Study of kinetics of organic reactions in a microwave-assisted flow-chemistry micro-reactor.
2. Analysis of organic contaminants in environmental samples.

Marine Chemistry

Field of research: Iron and other trace elements Biogeochemistry



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Project suggestions

1. *Improvement the analytical methods for iron determination in seawater*

Iron is an essential micronutrient for microbial organisms (bacteria and phytoplankton) in oceans. Iron is a limiting nutrient in almost 40 % of the Ocean, especially in the Antarctic waters and most of the Southern Ocean. It is one of the key element which has important role for regulation of the atmospheric CO₂ hence Climate of the Earth.

Determination of iron and its forms in seawater is a challenging task. The student will test various factors to improve the determination of the iron by using Sea-FAS pre-concentration instrument and High Resolution Inductively Coupled Plasma - Mass Spectrometry (HR-ICP-MS)

2. *Impact of CO₂ seepage from subsea-bed CO₂ storage sites on the biogeochemistry of trace elements at the sediment –water interface*

This project will be part of two projects (an EEA project and a NFR projects with international partners). The task is to follow the mobilization of the different trace elements (both toxic and bio-essential elements) mobility and distribution of the surface sediment. Multi analytical techniques will be used to determine the distribution and transformation of elements (i.e. Sea-fast pre-concentration technique, ICP-MS, sediment sequential extraction etc).

3. *Impact of CO₂ seepage from subsea-bed CO₂ storage sites on the biogeochemistry of dissolved organic matter (DOM) –metabolites at the sediment –water interface*

This project will be part of two projects (an EEA project and a NFR projects with international partners). The task is to follow the mobilization and characterization of the organic matter, their mobility and distribution at the sediment- water interface. Multi analytical techniques will be used to determine the distribution and transformation of DOM (i.e. Synapt G2-S Q-TOF and Fourier transform ion cyclotron resonance mass spectrometry (FTICR-MS))

Environmental Chemistry

Development and Application of State-of-the-Art LC-MS/MS Environmental Methods for the Measurement of Emerging Pollutants



Associate Professor, Alexandros Asimakopoulos
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Project suggestions

1) Develop a multi-residue method for benzotriazoles and benzothiazoles analysis, measure sediment samples from Trondheimfjord and perform environmental assessment (co-supervisor: Øyvind Mikkelsen)*.

1,2,3-Benzotriazoles (BTRs) and 1,3-benzothiazoles (BTHs) are high production volume environmental pollutants. Their application in deicing/anti-icing fluids, chemotherapeutics (antitumor agents), and in rubber manufacturing has been reported. In this project, a liquid chromatography–tandem mass spectrometry (LC–ESI(+)-MS/MS) method will be developed and applied for the quantification of eight aforementioned BTRs and BTHs, in 50 sediment samples from Trondheimfjord, Norway, in order to assess the occurrence and profile of these pollutants. Professor Øyvind Mikkelsen will provide sediment samples and organize sampling campaigns, if needed, for sample collection.

2) Develop a multi-residue method for benzophenone-type UV filters (BP-UV filters analysis) analysis, measure sediment samples from Trondheimfjord and perform environmental assessment (co-supervisor: Øyvind Mikkelsen)*.

BP-UV filters are used as sunscreen agents in personal care products for the protection of skin and hair from UV irradiation. Most of them end up in the environment as pollutants. In this project, a liquid chromatography–tandem mass spectrometry (LC–ESI(-)-MS/MS) method will be developed and applied for the quantification of six BP-UV filters in 50 sediment samples from Trondheimfjord, Norway, in order to assess the occurrence and profile of these pollutants. Professor Øyvind Mikkelsen will provide sediment samples and organize sampling campaigns, if needed, for sample collection.

*The experienced project team has its core at the Department of Chemistry, The Norwegian University of Science and Technology (NTNU), Trondheim, Norway. The master student will work under the guidance of one PhD student (Kristine Vike) and a post-doc researcher (Shazia N. Aslam). The work from the aforementioned projects will be disseminated in a peer-reviewed scientific journal (s).

3) Determination of particle and dissolved organic carbon in seawater and sediment pore water is important to understand the distribution of carbon (co-supervisor: Murat V. Ardelan)#.

This is essential to understand one of the main controlling mechanisms of atmospheric CO₂; Carbon export from atmosphere into the deep water and sediment. This project will be part of two projects (an E.U. and NFR projects with international partners). The task is to follow the mobilization and characterization of the organic matter, and their mobility and distribution at the sediment-water interface and sedimentary bed. Multi analytical techniques will be used to determine the distribution and transformation of DOM (e.g. LC-MS/MS, CDOM, FDOM). Sampling campaigns will be organized by Murat V. Ardelan.

#The experienced project team has its core at the Department of Chemistry, The Norwegian University of Science and Technology (NTNU), Trondheim, Norway. The master student will work under the guidance of two PhD students. The work from the aforementioned projects will be disseminated in a peer-reviewed scientific journal (s).

Department of Chemistry/PoreLab: Non-Equilibrium Thermodynamics

Porous media for renewable energy technology and nanotechnology.



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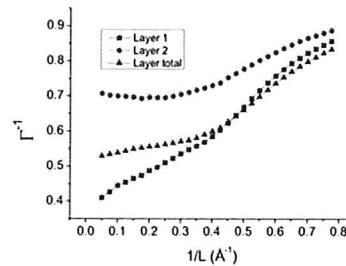
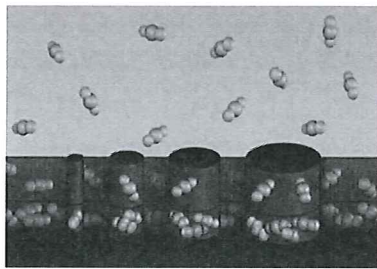
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Master project suggestions. The group of non-equilibrium thermodynamics at Department of Chemistry is part of PoreLab Center of Excellence, an interdisciplinary team between Department of Physics, Department of Chemistry, and Department of Geoscience and Petroleum at NTNU, and Department of Physics at UiO. The Center offers master projects linked to ongoing research projects (PhD projects). The master projects can be experimental (proposal 2) or computational, depending on the student's interest (please discuss). Computational projects are frequently molecular simulations (see proposals 3 - 6), but also process simulations are relevant (proposal 1). Smaller or larger parts of the project can be done abroad (Spain, Germany, The Netherlands, England, France, US). The list should be regarded as examples.

1. **Nature-inspired chemical process design.** We study the entropy production in the nose of various animals in the arctic and test the hypothesis that nose has evolved to keep as much of the body heat and water as possible. What could be the bearing of this on the design of heat recuperator in a house? The student will do process simulations for simple models and link the results to the knowledge of nature.
2. **Thermoelectric energy conversion.** We study the ability of systems of ion exchange membranes and salt solutions, to better see how the system can exploit waste heat for power generation. Transport properties need be measured for this purpose. The performance of the generator can then be modelled. The student will measure Seebeck coefficients in the laboratory under controlled conditions and thereby enable analyses or waste heat power generation.

3. **Simulations of thermodynamic data and transport properties for thin film technologies.**

We have invented a new way to find properties of small systems (the Small Systems Method, SSM), knowing the behavior in the ordinary bulk. The SSM is an efficient way to determine properties of atomic-scale properties. This may allow us to study properties of small systems, for instance the thermodynamic factor Γ (right) for CO_2 adsorbed on graphite (left). The student will apply the SSM in molecular dynamics simulations of systems relevant for PoreLab (to be discussed).



4. **Coupled transport of heat and mass in porous media.** Most measurements of the Soret effect (component separation driven by a temperature gradient) are made in bulk liquid or gas. Important processes, such as water transport in membranes and hydrocarbon transport in oil reservoirs, occur, however, in porous media. It has been shown that a porous medium can modify the separation efficiency [1], but the atomic mechanisms are not well understood. This project aims to examine the role of molecular interactions between fluid and porous medium (wettability, pore size, fluid composition, etc.) on the Soret effect. The student will do non-equilibrium molecular dynamics simulations and combine the results with non-equilibrium thermodynamics.
5. **Effect of wettability and fluid viscosity on single-phase flow in a porous medium.** Experimentally, it is well known that increased fluid viscosity decreases the flow rate in a porous medium for a given pressure drop. The effect of wettability (in one-phase flow) is less clear. This can be examined by doing molecular dynamics simulations of a fluid in a porous matrix. The student will do such non-equilibrium simulations and systematically relate the flowrate to fluid- and matrix properties in order to map the relationship(s).
6. **Relating the permeability and porosity of a porous medium.** The permeability of a porous medium is extremely important for process design, whether the process is water production from an aquifer, oil- or gas production from a reservoir, or any other process involving flow in a porous medium. It is easier to measure the porosity than the permeability, and many correlations between the two exist. However, the permeability depends on many other properties of the porous medium, such as the pore structure and the wettability. The student will in this project do molecular dynamics simulations to examine how the permeability depends on very controlled properties of a simple model for a porous medium.

[1] V. M. Barragan og S. Kjelstrup, «Thermo-osmosis in Membrane Systems: A Review,» *J. Non-Equilib. Thermodyn.*, vol. in press, 2017.

Surface analysis of pretreated aluminium

Hovedveileder: Andreas Erbe

Medveileder(e): Kemal Nisancioglu, Otto Lunder, Thomas Hentschel (Hydro Aluminium Rolled Products R&D Bonn)

Beskrivelse:

The usage of aluminium sheet for car bodies is rapidly increasing. For such applications, requirements regarding surface appearance and corrosion resistance are extremely high. Corrosion resistance is the result of a complex interaction of alloy, pre-treatment and coating.

Goal of this project is to achieve a better understanding of how surface chemistry controls corrosion resistance. In addition, it would be desirable to develop an electrochemical technique to estimate corrosion resistance, and to evaluate corrosion resistance in a simple manner.

The task of the candidate in this project are characterization of differently pretreated sheet samples by means of chemical analysis, electron or optical microscopy, electrochemical analysis of the samples in a relevant electrolyte (e. g., by voltammetry, electrochemical impedance spectroscopy), and corrosion testing. Final goal is to achieve a correlation of surface chemistry and corrosion resistance.

There is the possibility to do part or all of the work on this topic at Hydro Rolled Products Research and Development facilities, Bonn, Germany. This would, however, require a certain level of German language skills from the candidate.

Krav til kvalifikasjoner/forutsetninger:

Course TMT4255 Corrosion and Corrosion Protection or equivalent. In case of interest to work at Hydro Rolled Products R&D, certain German language skills are required.

Mulighet for sommerjobb: Ja Nei [to be confirmed]

Feil og reproduserbarhet i klassiske simuleringer

Hovedveileder: Sondre K. Schnell

Medveileder(e): [Click here to enter text.](#)

Beskrivelse:

Klassiske molekyl simuleringer har blitt brukt siden 60-tallet for å modellere termodynamiske- og transport egenskaper fra molekylære system. Nye metoder gjør at vi kan modellere alt fra enkle gass-systemer til DNA. I løpet av de siste 50 årene har regnekraften økt med flere størrelsesordener, og simuleringer som før krevde uker eller måneder på super-datamaskiner kan i dag gjøres på noen minutter på en vanlig laptop. I tillegg har algoritmer og programmer blitt standardisert, og arbeid som før kunne kreve uker kan nå gjøres på en ettermiddag.

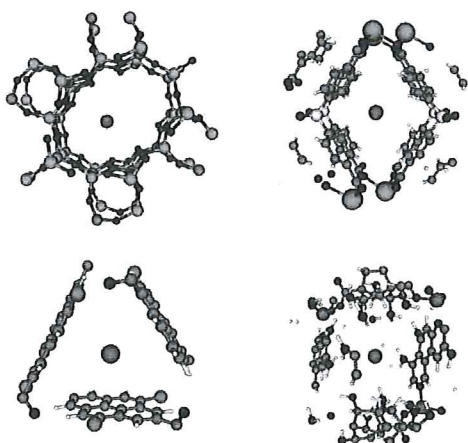


FIGURE 4 ADSORPSJON I PORØSE MATERIALER.

I dette prosjektet vil vi studere hvordan denne standardiseringen har gitt bedre og mer pålitelig data. Dette kan gjøres ved å se på noen utvalgte publikasjoner fra de siste 20 årene, og studere data oppgitt i disse arbeidene. Det er særlig adsorpsjons og transport modeller som kan enkelt etterprøves.

Det er ønskelig at dette skal resultere i ett system som muliggjør mer etterprøvbare resultater, og at studenten skal kunne foreslå et system for hvordan simuleringer metoder skal dokumenteres, og resultater presenteres på en slik måte at de kan etterprøves i framtiden.

Kinetisk Monte Carlo for transport i system med høy tetthet

Hovedveileder: Sondre K. Schnell

Medveileder(e): [Click here to enter text.](#)

Beskrivelse:

Diffusjon i system med høy tetthet er en sen prosess. Vanlige diffusjonskoeffisienter ligger mellom 10^{-10} og $10^{-20} \text{ m}^2\text{s}^{-1}$. Diffusjon i gass og væsker er vanligvis så kjapp at den kan studeres med klassiske molekyl simuleringer (opp til 100 ns). Den sakte diffusjonen som ofte observeres i systemer med høy tetthet (vanligvis $\gg 100$ ns) gjør at klassiske molekyl dynamikk simuleringer er uegnet for å studere transport fenomener i slike systemer.

En måte å omgå denne begrensningen i klassiske simuleringer er å bruke kinetiske Monte Carlo (kMC) simuleringer til å beskrive transport i molekylære systemer. kMC er en teknikk der de mulige endringene i systemet kartlegges på forhånd, og systemets endring mellom disse tilstandene simuleres, der den karakteristiske tiden en partikkel trenger for å flytte seg gjennom systemet måles og brukes for å bestemme diffusjonskoeffisienten.

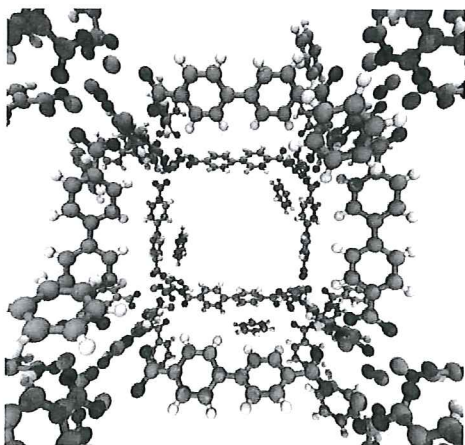


FIGURE 5 MOF-5 METAL-ORGANISK GITTER. EN PORØS STRUKTUR DER DIFFUSJON ER HINDRET PGA. INTERAKSJON MED OMKRINGLIGGENDE GITTER.

samme system.

I dette prosjektet vil vi bruke kMC simuleringer til å studere diffusjon i grafitt. Vi vil først fokusere på transporten av litium ioner. En modell av grafitt må lages, og et kMC program vil brukes for å kartlegge transporten av ioner. Om tiden tillater så vil modellen utvides til å takle transport av flere typer ioner i

Kinetisk Monte Carlo for vekst av overflater

Hovedveileder: Sondre K. Schnell

Medveileder(e): 1 PhD-student

Beskrivelse:

Kinetiske Monte Carlo (kMC) simuleringer kan brukes for å studere systemer som endrer seg over lang tid. Dette er gjerne systemer der det er store energi-barriere, eller dynamikken er så sen at det ikke er realistisk å se endringer innen rimelig tid. Et system som utvikler seg på denne måten er krystaller som vokser i en løsning. I dette prosjektet vil vi studere hvordan en overflate av en enkel krystall vokser under forskjellige betingelser. Som et utgangspunkt vil vi bruke en krystall av Argon. Dette skal generaliseres og utvides til mer kompliserte system, for eksempel vekst av is-krystaller under forskjellige betingelser.

Atomistiske simuleringer av batterier

Hovedveileder: Sondre K. Schnell

Medveileder(e): PhD-student

Beskrivelse:

Batterier er en svært viktig energibærer. Elektrokjemiske celler i form a Li-ion batterier brukes allerede i dag som lagringsmetode for energi i transport sektoren. Det er flere problemstillinger som fremdeles må adresseres for å øke kapasiteten og levetiden til elektrokjemiske celler.

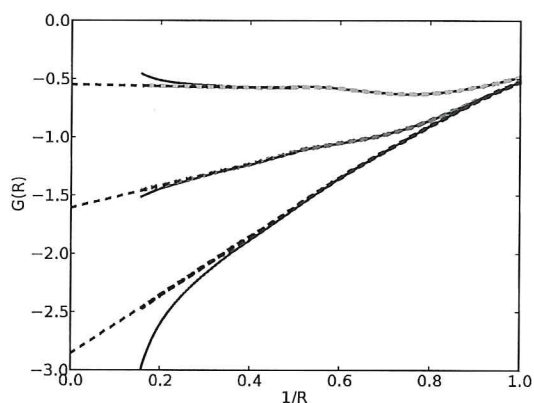


FIGURE 6 KIRKWOOD-BUFF TEORI KAN BRUKES FOR Å RELATERE FICK OG MAXWELL-STEFAN DIFFUSJON. VI BRUKER DEN NYLIG UTVIKLEDE SMÅ-SYSTEMERS METODE FOR Å BESTEMME DENNE SAMMENHENGEN I ELEKTROLYTTEN.

I dette prosjektet vil vi fokusere på egenskaper til elektrolytten i Mg-ion batterier. Elektrolytten har betydning for flere egenskaper ved batterier, blant annet tiden det tar å lade opp/ut batteriet. Det er

essensielt å forstå hvordan ioner interagerer med hverandre molekyler i elektrolytten. Vi vil bruke molekyl-dynamikk simuleringer til å studere transport av Mg-ioner i noen av de vanligste elektrolytt-løsningene. Vi vil bruke Kirkwood-Buff teori for å studere sammenhengen mellom Fick og Maxwell-Stefan diffusjon. Vi vil vurdere hvordan elektriske felt påvirker transporten.

A new generation of bipolar plates for PEM fuel cells

Hovedveileder: Frode Seland (frodesel@ntnu.no)

Medveileder(e): Katie McCay (katie.mccay@ntnu.no), Ole Edvard Kongstein (SINTEF)

Beskrivelse:

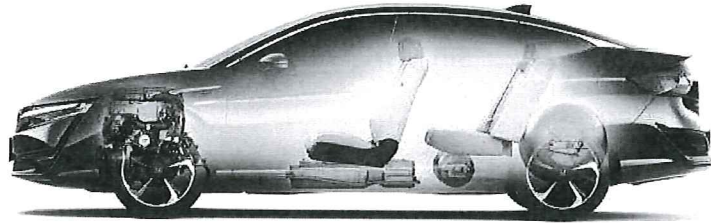
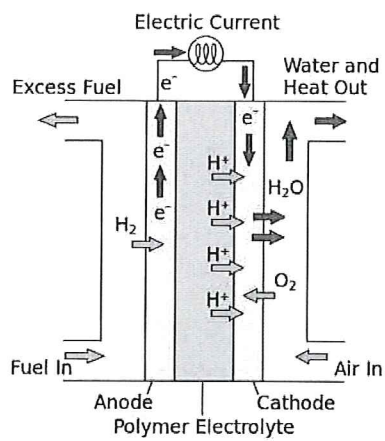
Proton exchange membrane (PEM) fuel cells are seen as one of the futures of green energy. They provide lightweight, high energy density, clean power with the only by-product being water¹. Many motor companies (Toyota, Honda, Mercedes, Ford) are currently developing fuel cell vehicles (FCVs), and the sector is estimated to reach up to 2.2 billion USD by 2022².

Bipolar plates are a key component within a PEM fuel cell stack, with roles such as electron transfer, fuel and waste transport, and stack support³. However, stainless steel as a bipolar plate material suffers from poor corrosion properties, with a non-conductive oxide layer forming and hindering electron transport⁴. By coating these plates with non-corrosive but conductive materials, their lifetime can be dramatically extended. This makes PEM stacks cheaper and more reliable, and more suitable for industrial use.

This project builds on previous successful masters project collaborations with SINTEF MK, and will have close contact on a day-to-day basis with PhD thesis work. It will continue work coating bipolar plates via electrodeposition. A number of parameters such as electroplating deposition current, thickness and then hot-pressing procedure can be varied to find the optimum synthesis method. Analysis will be performed using contact resistance measurements and ex-situ electrochemical techniques such as linear sweep voltammetry and chronoamperometry. Surfaces will also be looked at using the SEM. In-situ characterization of the fuel cell at various operating conditions like temperature, humidity and fuel composition will be relevant in a newly established collaboration with Toyota.

The overall aim is to determine how the coated plates would survive within the fuel cell environment and to compare against current commercially available plates.

Interested students from both electrochemistry and materials science backgrounds are encouraged to contact Katie McCay and Frode Seland with any questions. Additional tasks allowing for more than one student within this topic will be arranged for, if relevant.



1. A SCHEMATIC DIAGRAM OF A PEM FUEL CELL 2. THE HONDA CLARITY FUEL CELL CAR

1. F. Barbir, *PEM Fuel Cells*, Elsevier, 2013
2. <https://www.alliedmarketresearch.com/fuel-cell-market>
3. R. a. Antunes, M. C. L. Oliveira, G. Ett, and V. Ett, *Int. J. Hydrogen Energy*, 2010, **35**, 3632–3647
4. K. Feng, G. Wu, Z. Li, X. Cai and P. Chu, *Int. J. Hydrogen Energy*, 2011, **36**, 13032-13042

Effekt av mangan på DSA elektroder under oksygenutvikling

Hovedveileder: Frode Seland (frodesel@ntnu.no)

Medveileder(e): Siri Marie Skaftun (siri.m.skaftun@ntnu.no)

Beskrivelse:

I Norge produseres sink via vandig elektrolyse i temperert svovelsyreelektrolytt ved Bolidens anlegg i Odda, som regnes som et av de mest energieffektive sinkverkene i verden. Under elektrolyse feller man ut sink på aluminiumskatoder gjennom reduksjon av sinkioner og oksygen-gass på blyanoder. Sink høstes dermed jevnlig ved stripping av sinkplatene fra aluminiumsplatene. I elektrolytten foreligger ulike elementer (fluorioner, jernioner, manganioner, osv.), som påvirker både effektivitet, sinkkvalitet, strømbytte og levetid til elektrodene. Tilstedeværelsen av manganioner i elektrolytten vil kunne gi avsetninger av manganoksid på blyanodene, parallelt med gassutvikling. Et av problemene som følge av manganoksidutfellingen er at elektrolyseprosessen må jevnlig stanses for å "rense" blyelektrodene for utfelt manganoksid. I tillegg til manganoksidutfelling løses også noe bly ved høye positive potensialer og selve blyelektroden må byttes ut etter noen års drift. Bly har i tillegg dårlige katalytiske egenskaper for oksygenutvikling, som gjør at man bruker mer energi for hver kilo sink produsert. Optimalisering av driften er en nødvendighet i dagens elektrolyseindustri som opplever knallhard konkurranse med lave sinkpriser.

I tillegg til dårlige katalytiske egenskaper til bly, er også bly uønsket som anodemateriale på grunn av negative helseeffekter forbundet med langvarig eksponering mot bly. Elektrolyseindustrien ønsker derfor å gå over til bruk av dimensjonsstabile anoder (DSA) bestående av titansubstrat belagt med edelmetalloksider (rutenium- og iridiumoksid). Disse elektrodene er godt kjent innen oksygenutvikling for vannelektrolyse i surt miljø, et tema elektrokjemigruppen ved institutt for materialteknologi har arbeidet målrettet med over lang tid.

I denne oppgaven ønsker man å studere ulike DSA elektroder og effekten av tilstedeværelsen av mangan i svovelsyreelektrolytten under oksygenutvikling. Manganutfellingen vil studeres med konvensjonelle elektrokjemiske metoder som potensialtrinn og syklisk voltametri, i tillegg til mer avanserte metoder som elektrokjemisk kvartskrystallvekt (EQCM). Ulike binære oksider (iridium og tantaloksid) vil bli syntetisert og karakterisert før påføring på egnet substrat og testet elektrokjemisk. SEM/XRD vil benyttes for å studere og karakterisere katalysatorene i tillegg til utfelt manganoksid som vil dannes ved ulike betingelser som strømtetthet, temperatur, pH og Mn^{2+} konsentrasjon. Denne prosjektoppgaven vil være av interesse for flere andre prosjekter ved faggruppen og vil følges opp tett, på daglig basis, av stipendiat Siri Marie Skaftun.

Ni Based Multi-metallic Nanoparticles for Alkaline Anion Exchange Membrane Fuel Cell

Hovedveileder: Svein Sunde

Medveileder(e): Post doc Maidhily Manikandan, Alejandro Oyarce Barnett (SINTEF),
Frode Seland

Beskrivelse:

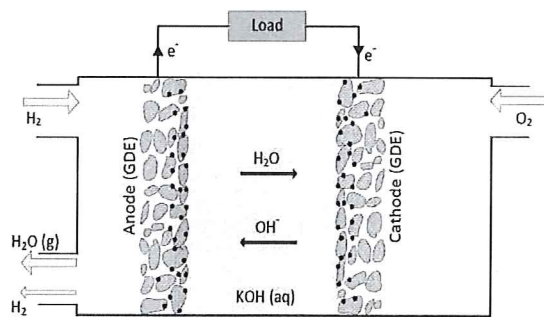
The rising global energy requirements and the environmental concerns demand much sustainable form of energy, which do not contribute to the global warming. Fuel cells are one of the efficient and clean energy conversion devices that convert chemical energy of a fuel to electrical energy. Alkaline Fuel Cell (AFCs) became one of the sustainable and reliable energy sources ever since it was used in the 1960's Apollo space mission ¹.

Pt group metals (PGM) dispersed on a conductive carbon supports are the state of the art electro catalysts for low temperature fuel cells. However, at the fuel cell anode side the hydrogen oxidation reaction (HOR) kinetics in alkaline media is ~100 times slower than that in acidic media. Therefore a high Pt loading may be required in order to achieve a comparable performance, whereas minimum Pt loading is enough to start the HOR reaction in acidic media². Hence, it is highly desirable to look for a the PGM free anode catalyst for the HOR in AFCs. Ni based alloys are one of the alternative choices since Raney Ni and some of the Ni based alloys have been found showing improved HOR activity³.

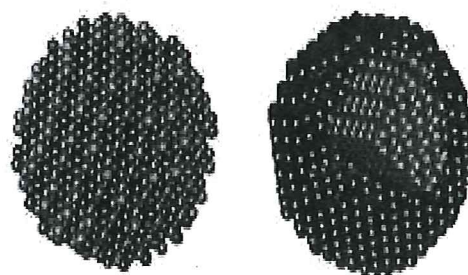
The aim of this project is to develop Ni-based bi or tri metallic nanoparticles for the HOR in AFCs. The master student will be working on the synthesis of nanoparticles with various compositions by a thermal reduction method. The structure, composition and crystallinity of the materials will be examined by various characterization techniques such as XRD, SEM and TEM. Electrochemical analysis such as cyclic voltammetry, linear sweep voltammetry and chronoamperometry will be used to evaluate the HOR activity and stability by use of a potentiostat. This project is running in collaboration with SINTEF and another two universities from Taiwan and Israel. The student will be on a day-to-day base interaction with a post doc.

The overall objective of this work is to find a suitable Ni based multi-metallic nanomaterials with better HOR activity as well as stability. The best catalyst will also be operated under the real fuel cell conditions. This project will lead to a Masters assignment/thesis.

Interested students from both electrochemistry and materials science backgrounds are encouraged to contact Maidhily Manikandan with any questions.



Schematic diagram of an Alkaline Fuel Cell



Representative images of an alloy and core shell

nanostructures

References

1. Perry, M.L, Fuller T.F, *J.Electrochem.Soc.* 149 (2002).
2. Zhuang, Z, Giles, S.A, Zheng, J, Jenness, G.R, Caratzoulas, S, Vlachos, D.G, Yan, Y *Nat. Commun.* 7 (2016).
3. Kenjo, T. *J. Electrochem. Soc.* 132 (1985)

Krav til kvalifikasjoner/forutsetninger:

Interesse for syntese av nanopartikler og strukturell karakterisering. Bakgrunn i elektrokjemi svarende til TMT4252 Elektrokjemi er en fordel.

Core/Shell catalyst nanoparticles for water electrolysis

Hovedveileder: Svein Sunde

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Beskrivelse:

An important step in the transition from fossil fuels towards renewable energy is the utilization of hydrogen as an energy carrier. Most of the hydrogen consumed today stem from catalytic steam-reforming or partial oxidation of fossil fuels. These processes adversely affect the on the environment due to concomitant production of carbon dioxide, among other things.

Water electrolysis, on the other hand, provides an environmentally benign method of hydrogen production. Several technologies exist, of which the classical alkaline process has been utilized industrially for more than hundred years. However, alkaline water electrolysis is considerably less efficient than what would be required for use in an energy system. The more recent and competing PEM technology, which employs a proton-conducting polymer electrolyte membrane (PEM), may provide substantial advantages in this respect. However, the PEM technology requires expensive catalysts both for the hydrogen evolution reaction (HER) at the cathode, which is catalyzed by platinum, and the oxygen evolution reaction (OER) on the anode which is catalyzed by iridium and ruthenium oxides. State-of-the art cathode catalysts are typically made by supporting nanoparticles of Pt on carbon, whereas the anode catalysts are frequently used unsupported. The HER is a facile reaction under the acidic conditions in the proton –conducting membrane, and is not associated with significant losses. In acidic media, the OER on the other hand leads to large efficiency losses, and with current technology high catalyst loadings of typically $3\text{mg}/\text{cm}^2$ of iridium oxide are required to keep energy consumption down.

Work at NTNU and in other research groups has demonstrated the possibility of employing anode catalysts in the form very thin layers, possible monolayers, of the catalyst on top of a cheaper substrate. Thus, by creating for example a core-shell structure, in which a thin layer of the catalyst metal oxide is deposited on a cheaper but stable substrate, one would achieve a high utilization of the catalysts, thus reducing cost and stretching resources of scarce and expensive metals such as iridium. Current work in the NTNU/SINTEF project with which this student project and master thesis is associated aims at significant reductions in catalyst loading in PEM water electrolyzers without compromising performance.

The aim of this project is thus to synthesize core-shell catalysts with iridium oxide shells at substrates such as nickel and copper. The catalysts will be characterized by various

characterization methods such as XRD and SEM/STEM. Electrochemical characterization by cyclic voltammetry and linear sweep voltammetry will also be a central part of the project.

The student project and master thesis will be performed under the direct guidance of a PhD student and in close collaboration with SINTEF in a research area of significant international interest.

Krav til kvalifikasjoner/forutsetninger:

Interesse for syntese av nanopartikler og strukturell karakterisering. Bakgrunn i elektrokjemi svarende til TMT4252 Elektrokjemi er en fordel.

MASTER STUDIES

MARINE CHEMISTRY & BIOGEOCHEMISTRY



Trace elements /micronutrients biogeochemistry

1- Studying iron uptake and growth rate of two different phytoplankton a) *prokaryote* (cyanobacteria) and b) *eukaryote* (Diatom)

Both cyanobacteria (blue-green algae) and diatoms are very important microbial organism for marine productivity, Nitrogen and Carbon cycles.

To study iron uptake of these microorganism may give crucial information for evolutionary mechanism of phytoplankton in marine systems.

Collaboration with Dept. of Biotechnology

In addition, we work together with **biotechnological researchers** to control genes, which are expected to be involved in a newly discovered iron uptake mechanisms. By comparing the growth rates and physiology of the mutants and the wild type under iron shortage we can draw important conclusion about the iron uptake mechanism.

Experiment : Phytoplankton cultures will be incubated with different iron forms and their growth rate and uptake rate of iron will be monitored. Different forms of iron in water and in cell will be determined



2- Improvement the analytical methods for iron and other trace element determination in seawater

a) *Multi analytical approach for Iron determination in seawater*
Iron is an essential micronutrient for microbial organisms (bacteria and phytoplankton) in oceans. Iron is a limiting nutrient in almost 40 % of the Ocean, especially in the Antarctic waters and most of the Southern Ocean. It is one of the key element which has important role for regulation of the atmospheric CO₂ hence Climate of the Earth.

Determination of iron and its forms in seawater is a challenging task. The student will test various factors to improve the determination of the iron by using Sea-FAST pre-concentration instrument and High Resolution Inductively Coupled Plasma - Mass Spectrometry (HR-ICP-MS) and Flow Injection Analysis (FIA)

b) Multi analytical approach for selected trace element (i.e. Mn, Co, Ni, Zn, Cu, Au, Cd, Pb, U and Ti) determination in seawater.

Some trace elements (TE) are essential as micronutrients for microbial organisms (bacteria and phytoplankton) in oceans. They are crucial in many vital enzymatic reactions. Some other trace elements are toxic for marine organism. Due to climate change and human made impact, the mobility, solubility hence bioavailability and toxicity of TE may be changing dramatically. It is, therefore, important to develop useful analytical techniques to monitor the changes in TE concentration in seawater and their roles in ecosystem.

Determination of iron and its forms in seawater is a challenging task. The student will test various factors to improve the determination of the iron by using Sea-FAST pre-concentration instrument and High Resolution Inductively Coupled Plasma - Mass Spectrometry (HR-ICP-MS) and Diffusive Gradient in Thin film (DGT) methods.

Ocean Acidification

Impact of CO₂ seepage from subsea-bed CO₂ storage sites on the biogeochemistry on the sediment-water interface



3- Trace and rare earth elements (REE) at the sediment –water interface

This work will be part of a NFR projects with international partners). The task is to follow the mobilization of the different trace elements (both toxic and bio-essential elements) mobility and distribution of the surface sediment. Multi analytical techniques will be used to determine the distribution and transformation of elements (i.e. Sea-fast pre-concentration technique, ICP-MS, sediment sequential extraction etc).

Experiment : Pressurized Titanium tank (Karl Erik TiTank) was developed specially to study the impact of CO₂ leakage on the marine ecosystem, is a unique experimental vessel. KE-TiTank offers us a continuous monitoring of CO₂ l impact on marine ecosystem under fully controlled seawater flow rate, various CO₂ fluxes, and various pressures (1 - 30 atm) conditions. Samples will be taken the ongoing experiment under 30 Collaboration with SINTEF

4 - Dissolved organic carbon (DOC) –determination and characterization

This project will be part of two projects (an EEA project and a NFR projects with international partners). The task is to follow the mobilization and characterization of the organic matter, their mobility and distribution at the sediment- water interface. Multi analytical techniques will be used to determine the distribution and transformation of DOC (i.e. Synapt G2-S Q-TOF, CDOM, FDOM).

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5 - Studying Fate of CaO addition and the effects of CaO (or Ca(OH)₂) to seawater and its impact on pH, alkalinity and dissolved inorganic carbon, DIC

Adding “quicklime” (calcium oxide, CaO) or “hydrated lime” (calcium hydroxide, Ca(OH)₂) in the seawater can neutralized H⁺ and increases alkalinity. That is why addition of CaO or Ca(OH)₂ to seawater have been suggested as mitigation technique for Ocean Acidification and named as “Ocean liming” (OL) or “artificial ocean alkalization” (AOA) (Kheshgi 1995, Paguey and Zeebe, 2013, Renforth et al., 2013, Renforth and Kruger, 2013). This technique may help to capture extra CO₂ from atmosphere by Ocean. However, there is extremely limited knowledge and a great uncertainty on OL and AOA, especially their possible impacts on marine biogeochemistry and ecosystem (Cripps et al, 2013; Paguey and Zeebe, 2013; Feng et al, 2016)

Experiment : Addition of CaO (or Ca (OH)₂) to seawater with different pH and alkalinity. we can chose initial pH conditions (pre-industrial, modern and future scenarios that is (pH:8.2-8.3; 7.9-8.0 and 7.7-7.8 respectively). pH and alkalinity of the seawater can be adjusted by using either CO₂ gas bubbling or addition of a mineral acid with combination of NaHCO₃/Na₂CO₃.

Sampling can be done by short and long-term perspectives (minutes, hours and days)

Analysis & Techniques: pH, alkalinity will be measured by using the potentiometric or optical methods. pCO₂, and DIC (HCO₃⁻, CO₃⁻², CO₂) will be calculated by using CO₂Sys and SeaCarb programs.

CaO, Ca(OH)₂, CaCO₃ and other Ca, Mg carbonate species will be followed by XRD after filtration. Relevant total and dissolved elements will be measured by SeFast connected HR-ICP-MS

6- Studying the effects of CaO (or Ca(OH)₂) addition to seawater and its impact on marine microbial ecosystem :

The impact of CaO/ Ca(OH)₂ addition on the calcifying phytoplankton *Emiliana huxleyi*, EHUX, the most dominant species of coccolithophore in the oceans.

Since CaO/ Ca(OH)₂ will affect master variables of pH and alkalinity, this may also cause positive or negative impact on marine organism, their internal pH and may alter acid–base balance of some marine organism. To test this hypothesis we proposed the following microcosm experiment.

Experiment : Addition of CaO (or Ca (OH)₂) to microcosm culture with different pH and alkalinity. we an chose pH condition for pre-industrial, modern and future scenarios that is (pH:8.2-8.3; 7.9-8.0 and 7.7-7.8 respectively) pH and alkalinity of the seawater can be

adjusted by using either CO₂ gas bubbling or mineral acid with combination of NaHCO₃/Na₂CO₃.

Sampling can be done by short and long term perspectives (minutes, hours and days). EHUX culture will be incubated under constant temperature and light, their growth rate and calc formation will be monitored.

Analysis & Techniques: pH, alkalinity will be measured by using potentiometric or optical methods. pCO₂, and DIC (HCO₃⁻, CO₃²⁻, CO₂) will be calculated by using CO₂Sys and SeaCarb programs. Calcium carbonate formation of EHUX will be monitored by electron microscopy.

CaO, Ca(OH)₂, CaCO₃ and other Ca, Mg carbonate species will be followed by XRD after filtration. Relevant total and dissolved elements will be measured by SeFast connected HR-ICP-MS. Analysis of dissolved fraction (< 0.2 μm): Techniques : HR-ICP-MS

CO₂/ Carbon cycle :

Characterization of the organic carbon in seawater and surface sediments

Increasing CO₂ in the atmosphere is one of the main global environmental problems. Both greenhouse effects and ocean acidification are due to accumulation of CO₂ in the atmosphere. It is critical to control CO₂ increase in the atmosphere. Oceanic processes are important for removal of CO₂ and control its level in the atmosphere by photosynthesis and eventually by exporting biologically fixed CO₂ as forms of dissolved and particulate Organic Carbon (DOC/POC) into deep water and sediment.

It is important to follow the carbon export from surface water to the deep water and its fate. In this work we are going to collect DOC and POC in water column and sediment (pore water) to characterize whether they are labile or refractory for microbial decomposition. Multi analytical techniques will be used to determine the distribution and transformation of DOC and POC (i.e. Synapt G2-S Q-TOF, , NMR, CDOM, FDOM). Collaboration with Marine Biologist in Dept of Biology.

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Reactive Oxygen Species (ROS)

Role of plankton for H₂O₂ production in seawater

Hydrogen peroxide, H₂O₂ is one of the most dominant ROS in surface water. It is very strong oxidizing molecules and increase in concentration of , H₂O₂ is important stressors for biology, and have critical impact of many vital chemical process in seawater.

We are testing the role of grazing activities of different zooplankton on the production of , H₂O₂

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