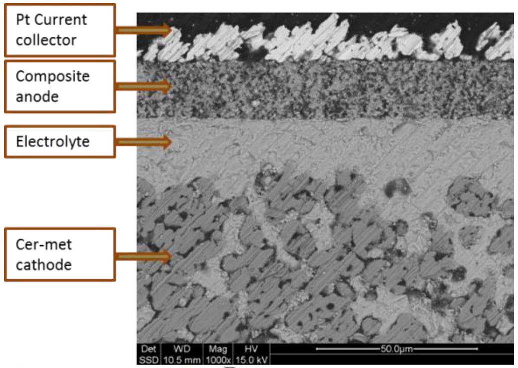
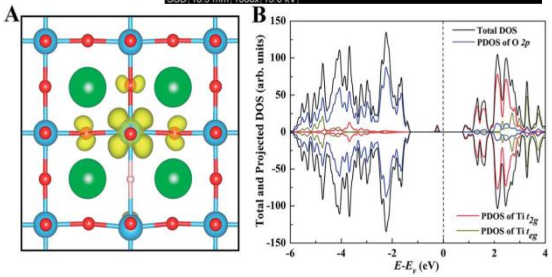
UiO : **Department of Chemistry**

University of Oslo



Elektrokjemi

Electrochemistry

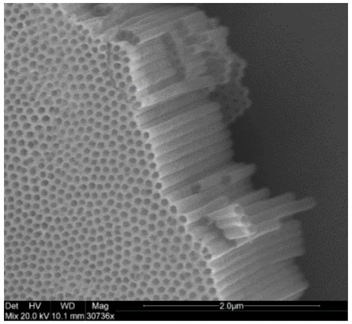


Truls Norby, Reidar Haugsrud, Jonathan Polfus

Electrochemistry: Research group and section at Department of Chemistry

FERMiO Functional Energy Related Materials in Oslo: Oslo Science Park

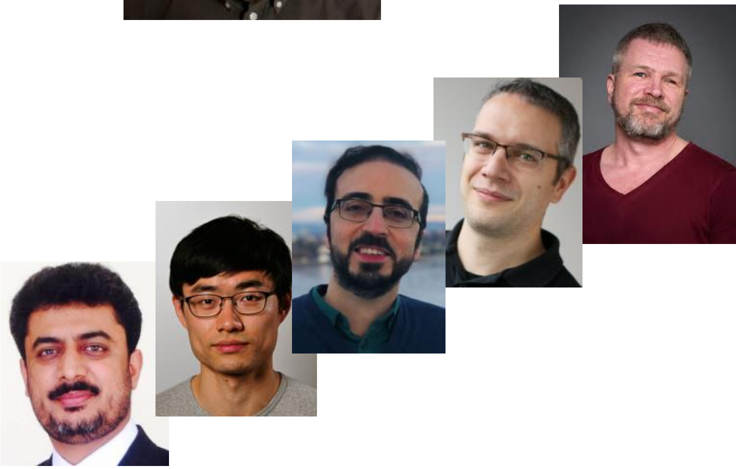
SMN Centre for Materials Science and Nanotechnology



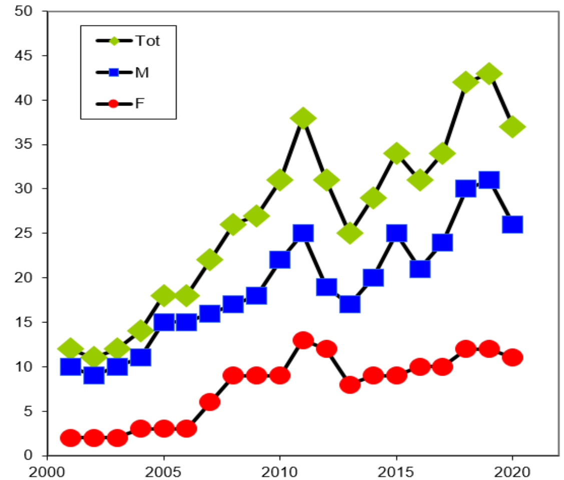
People in Electrochemistry

- Professors
  - Truls Norby truls.norby@kjemi.uio.no
  - Reidar Haugsrud reidar.haugsrud@kjemi.uio.no
  - Jonathan Polfus jonathan.polfus@kjemi.uio.no

- Staff researchers
  - Ragnar Strandbakke
  - Athanasios “Sakis” Chatzitakis
  - A. Masoud Dayaghi
  - Xin Liu
  - Asif Mahmood



  - 5 post-doc researchers
  - 10 PhD + 10 MSc students
  - Technical: Oddvar Dyrlie
  - Administrative: Xuemei Cui
  - BSc project students, visitors, interns



Master students

2019-2021

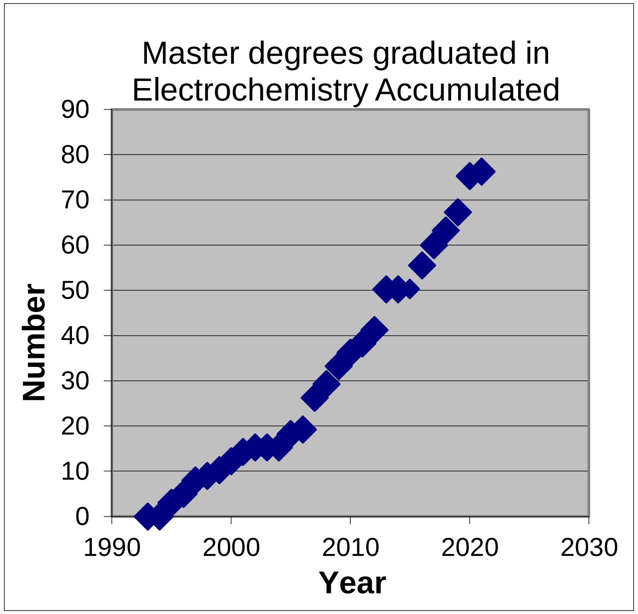
- Jonina Gudmundsdottir — Electrocatalysis — Sakis+T
- Tord Svee — Proton ceramics — Truls (T)
- Erik Alsgaard — Heterointerfaces — Truls
- Visa Mäntysalo — Defects & transport — Reidar
- Egil S. Køller — Thermoelectrics — Truls
- Lorenzo Caprani — Proton conduction — Masoud+T

2020-2022

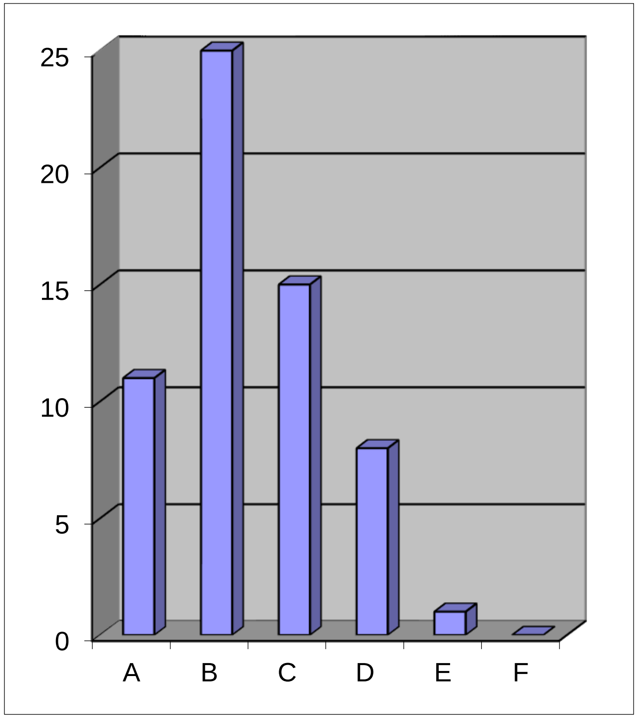
- Stine Roen — Proton ceramic electrodes — Ragnar+T
- Henrik Petlund — Electrocatalysis — Sakis+T
- Haider Abbas — New solid-state electrolyte — Reidar
- Sjur Storhaug — Proton ceramic electrolyte — Reidar
- Henry Chen — Proton ceramic electrolyte — Masoud+T

2021-2023

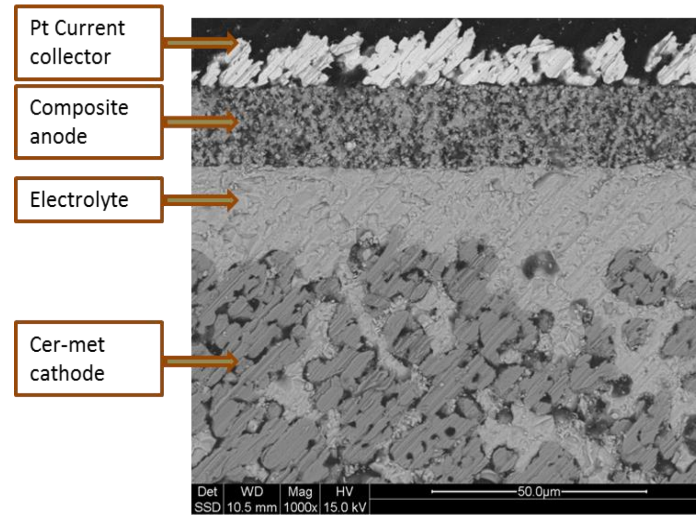
- **YOU ☺** — You+we choose together ☺ — We ☺



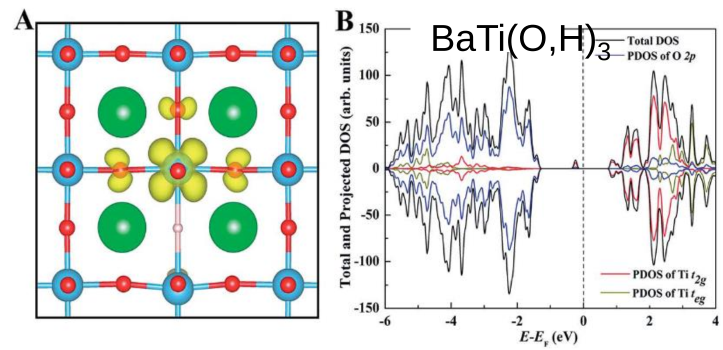
5 of 50 (10%) drop out. 90% pass



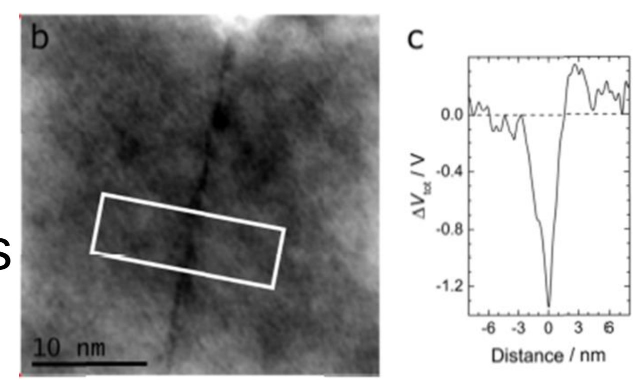
Electrochemistry: Fundamentals



- Properties of inorganic materials; thermodynamics and kinetics
- Structure and defects



- Diffusion, conductivity, reactions
- Nanoscopy
- Interfaces: Grain boundaries, surfaces, electrodes
- Physical chemistry – chemistry and physics



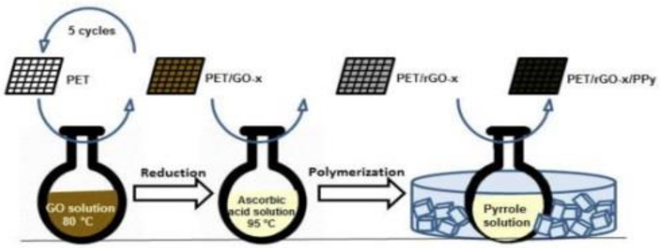
Electrochemistry: Methods

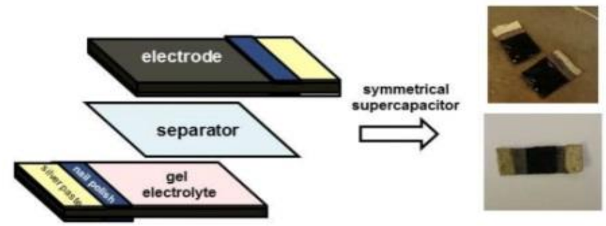
- Synthesis and fabrication
  - Wet chemical and solid-state synthesis
  - Fabrication, sintering
  - Film deposition
    - Pulsed Laser Deposition (PLD)

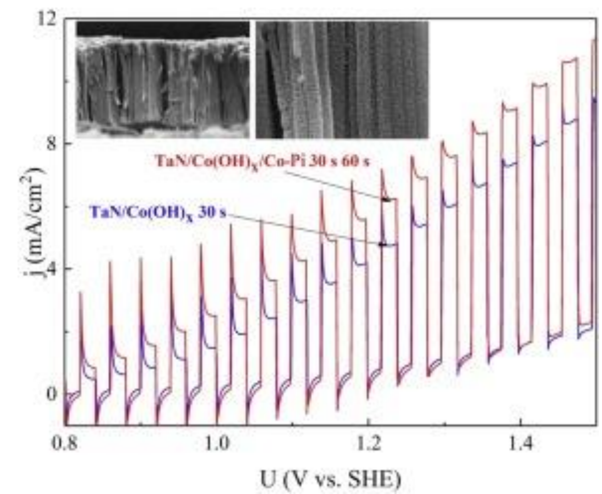
- Characterisation
  - XRD, SEM, (+TEM/ETEM, ToF-SIMS, ND, XPS, …)

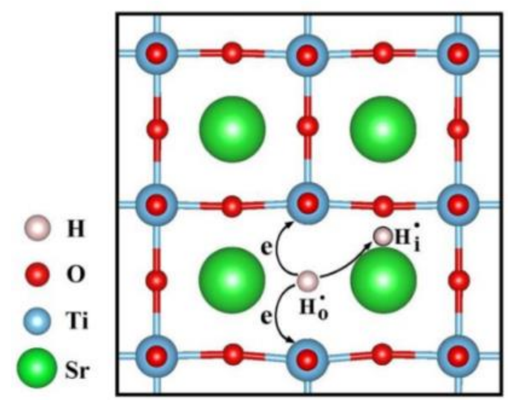
- Measurements
  - Electrical and thermoelectric properties
  - Electrocatalytic and photoelectrocatalytic properties
  - Thermogravimetry
  - Diffusion and kinetics
  - Performance of fuel cells and electrolysers
  - Solar water splitting and photosynthesis
  - Controlled temperature and atmospheres

- Theory and computational
  - Mathematics and computers
  - Atomistic simulations



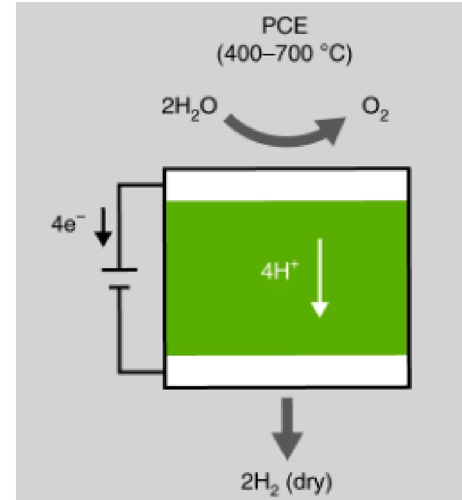


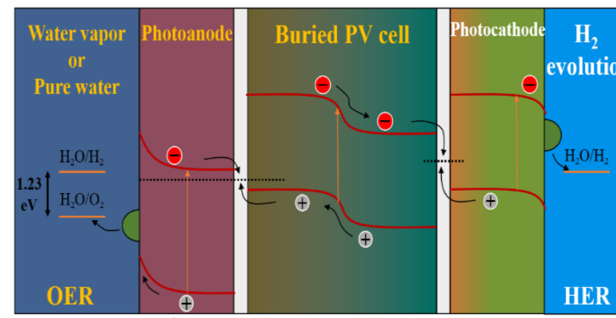


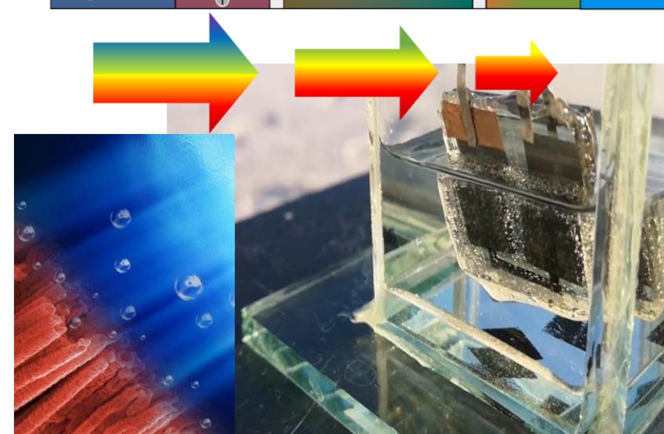


Electrochemistry: Applications

- Hydrogen
  - Fuel cells, electrolysers
  - Natural gas reforming, upgrade, dehydrogenation, etc.
  - Ammonia as H_2 carrier: Direct ammonia fuel cells
- Carbon capture (CCS)
  - Mixed conducting membranes for O_2, H_2, CO_2
- Heat recovery
  - Thermoelectrics
- Artificial photosynthesis
  - Nanomaterials, bionano, biocatalysts (enzymes)
- Novel electronics
  - Bottom-up fabrication, extreme conditions, AI, …







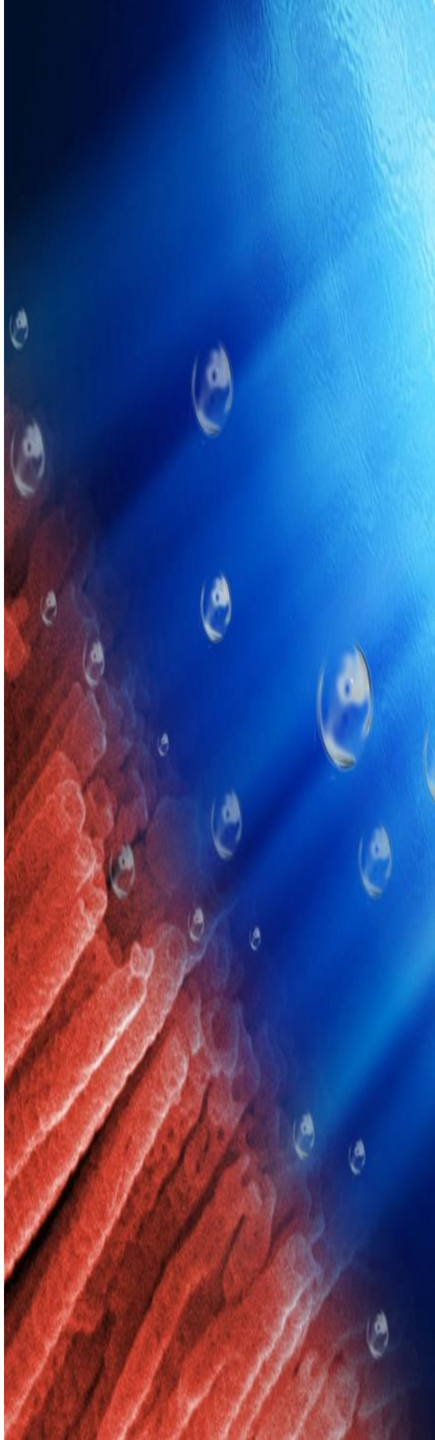
FERMiO

Projects and background

- We accept students from bachelor programs
  - Kjemi og biokjemi
  - Materialvitenskap for energi- og nanoteknologi (MENT)

- Bachelor projects
- Master projects

- Required background
  - None special
- Recommended background
  - Skills and interest in inorganic chemistry and/or physical chemistry
- Suggested courses
  - KJM3110 Electrochemistry
  - KJM-MENA3120 Inorganic Chemistry II
  - MENA3200 Energy materials



Examples of available BSc and MSc projects

Some explained in more detail in following slides

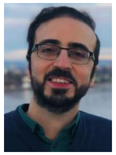
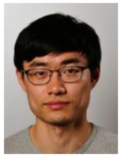
- Assoc. prof. Jonathan Polfus jonathan.polfus@kjemi.uio.no
  - 1. Proton and electron transfer at solid-solid electrochemical interfaces (MENT – MSc)
  - 2. Hydride ion diffusion in sub-stoichiometric titanium nitrides (MENT – MSc/BSc)
  - 3. Interlayer coupling in van der Waals heterostructures (KJM/MENT – BSc/MSc)

- Prof. Reidar Haugsrud reidar.haugsrud@kjemi.uio.no
  - 1. Mixed Anion metal Oxides (MAOs) – novel functional materials
  - 2. Ionic and mixed ionic-electronic conductors – materials for future energy technologies
  - 3. Surface kinetics/electrocatalysis – «everything starts at the surface

- Prof. Truls Norby truls.norby@kjemi.uio.no
  - 1. Novel catalysis for nitrogen fixation: Fertilizers
  - 2. Oxide thermoelectrics: Industrial waste heat recovery
  - 3. Novel p-n junctions for energy conversion

- Dr. Ragnar Strandbakke ragnar.strandbakke@kjemi.uio.no
  - Electrodes for proton ceramic fuel cells and electrolysers
- Dr. Athanasios “Sakis” Chatzitakis a.e.chatzitakis@smn.uio.no
  - Photoelectrochemistry: Novel electrocatalysts, solar hydrogen, artificial photosynthesis
- Drs. A. Masoud Dayaghi, Xin Liu, Asif Mahmood
  - More possibilities…




Career opportunities

- **Many of our Masters continue with PhD at UiO**
- **Others go to Norwegian and international companies and institutes**

BSc and MSc research projects at Electrochemistry supervised by Polfus et al.

Selected examples of MSc and BSc projects. Several of the projects have the possibility for collaboration with external partners such as SINTEF and Massachusetts Institute of Technology.

1. Proton and electron transfer at solid-solid electrochemical interfaces (MENA – MSc)

Electrochemical devices for clean energy technologies such as fuel cells and electrolyzers are in many cases limited by the performance of the electrodes. Due to the complexity of the electrode processes, involving mass transfer, charge transfer and diffusion, it is challenging to determine the rate limiting steps. The project focuses on the solid-solid interface between a state-of-the-art electrolyte (BaZrO3) and palladium which exhibits high bulk diffusivity of atomic hydrogen. This serves as model system to study proton and charge transfer mechanisms, and Pd has also shown great potential as an interfacial layer to boost electrode performance. The project can be combined experimental and computational. The experimental part includes sample preparation, electrode deposition including thin-film techniques, and electrochemical impedance spectroscopy (EIS). The computational part includes density functional theory (DFT) studies of the electrode interface and transfer mechanism of hydrogen between the materials.

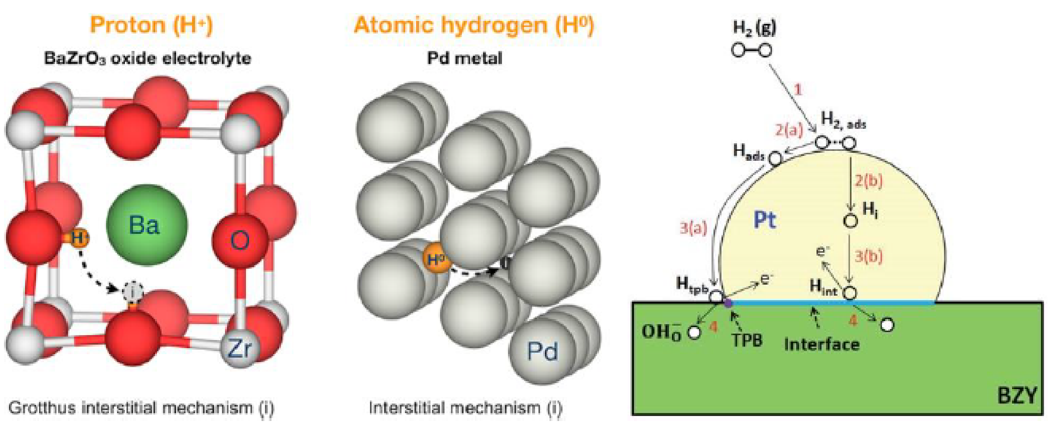


Figure 1: Chemical state and hydrogen migration mechanisms in the oxide electrolyte and Pd metal (left) and schematic view of gas-solid and solid-solid electrode reactions from Chen et al., J. Mater. Chem. A, 2020, 8, 12566.

2. Hydride ion diffusion in sub-stoichiometric titanium nitrides (MENA – MSc/BSc)

Fast diffusion of hydride ions in titanium nitrides (TiN_x) have been reported, but the mechanism is not yet understood. The project will address dissolution and transport of hydride ions in TiN_x as a function of composition, and grain boundaries will be considered as potential fast diffusion paths. The project can be combined experimental and computational. The computational part includes density functional theory (DFT) studies of the solubility and diffusion of hydride ions in bulk as well as at grain boundaries as a function of composition. The role nitrogen sub-stoichiometry and its impact on the electronic structure of the materials will be and important aspect. The experimental part has potential for many types of fabrication and characterization methods. For instance, instance isotope exchange of hydrogen in thin films deposited by pulsed laser deposition (PLD).

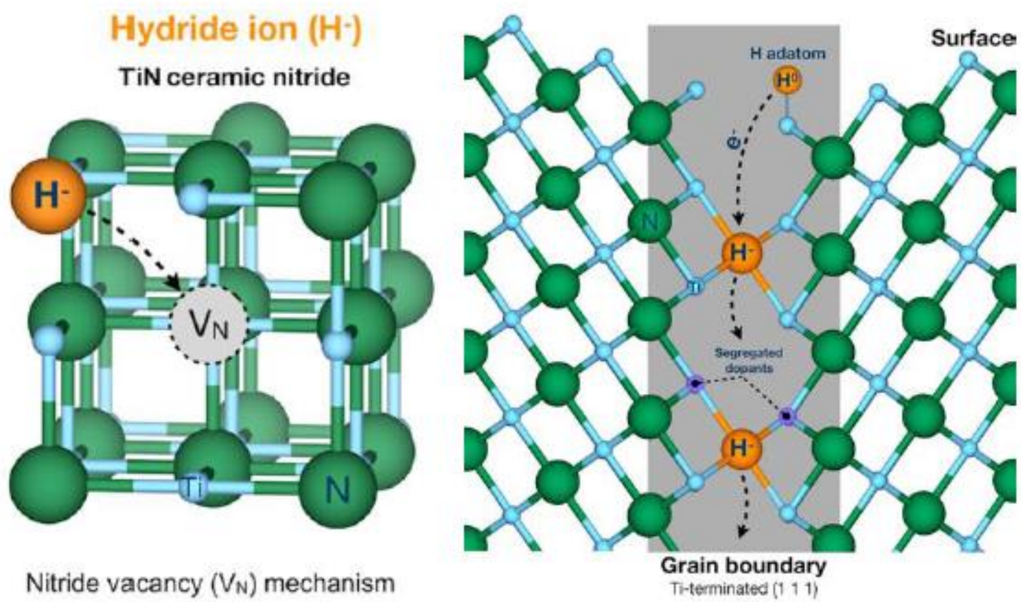


Figure 2: Hydride ions in TiN and hydrogen migration mechanisms along a grain boundary.

3. Interlayer coupling in van der Waals heterostructures (KJM/MENA – BSc/MSc)

Two-dimensional (2D) materials can be isolated as individual layers and stacked into artificial van der Waals (vdW) heterostructures that pave the way for a greater range of functionality in materials and devices including flexible electronics and sensors. The adhesion characteristics between 2D materials are not only of fundamental interest for understanding the bonding and properties of heterostructures, but also for the development of fabrication pathways involving transfer by vdW pick-up. While the vdW interactions themselves are principally independent of temperature, thermally induced ripples in 2D materials can give rise to a temperature-dependence in adhesion that is not yet well understood between different types of materials such as graphene, h-BN and MoS2. The adhesion characteristics will be studied by atomistic modelling and molecular dynamics simulations of vdW heterostructures at different temperatures.

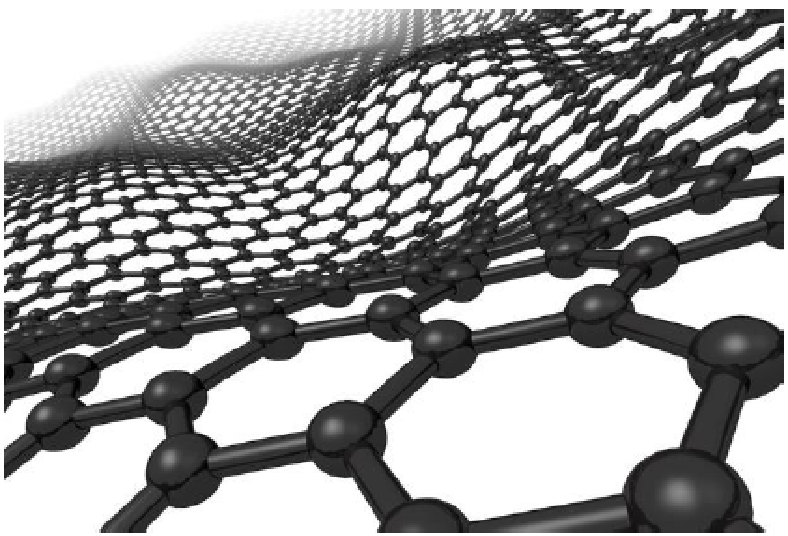
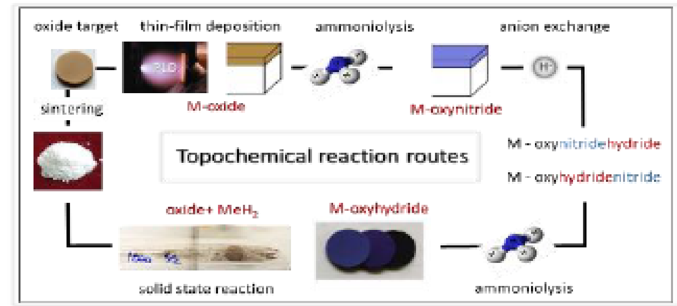


Figure 3: Thermally induced ripples in graphene (newatlas.com).

Energy related BSc and MSc research projects at Electrochemistry supervised by Haugsrud et al.

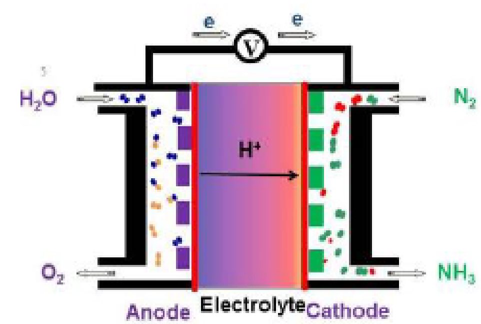
1. Mixed Anion metal Oxides (MAOs) – novel functional materials:

MAOs are families of metal oxides with one or more anion in addition to the oxide ion itself (e.g. $SrVHO_2$ and $BaCeH_xN_yO_{3-z}$). These are newly discovered solids with great potentials for design of functional properties relevant for applications in sustainable energy and chemical technologies. Figure illustrates cool synthesis routes.



2. Ionic and mixed ionic-electronic conductors – materials for future energy technologies:

Oxides conducting protons and/or oxide ions (ionic conductors), and mixed ionic and electronic(electron and electron holes), are central in development of sustainable energy interconversion technologies. This could typically be production of H_2 from "green" electricity by electrolysis and utilizing H_2 in a fuel cell, or as in the figure, for production of NH_3. Obviously, the development of these technologies is essential in a future carbon neutral society.

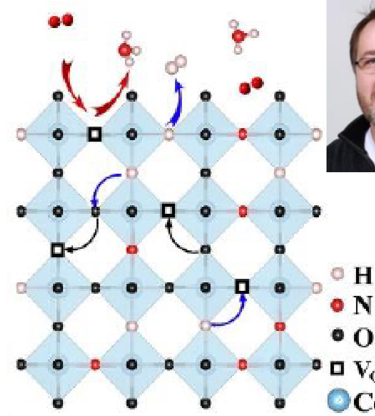


Anode: $3H_2O \rightarrow 6H^+ + 6e^- + \frac{3}{2}O_2$

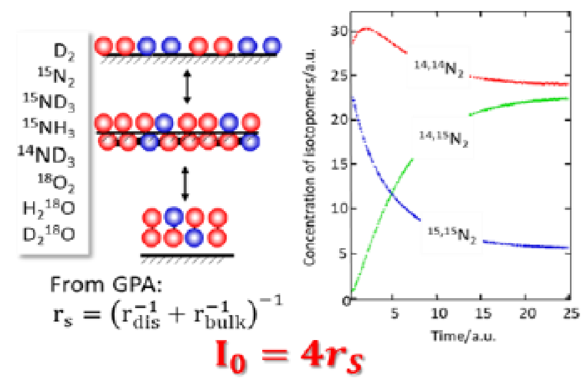
Cathode : $N_2 + 6H^+ + 6e^- \rightarrow 2NH_3$

3. Surface kinetics/electrocatalysis – «everything starts at the surface:

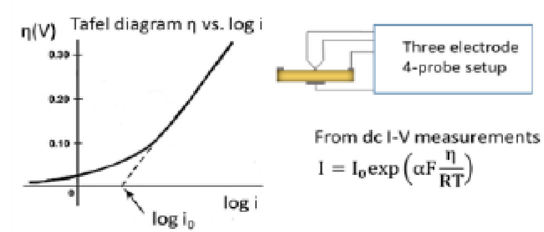
Heterogeneous reactions between the gas and solids relies on the kinetics of processes at the gas-solid interface. Developing this field of science related to the technologies described in (2) is essential to implement them in tomorrows. The figure illustrates how a surface may interact with H_2 and N_2, producing NH_3 in a mechanism where N_2 fixation relies partly on diffusion via anion vacancies.



A typical MSc project starts with synthesis of one or more material, but except for 1) MAOs, synthesis is not the major focus. It is rather characterization and understanding of functional properties, e.g. conductivity and transport properties, surface reactions, kinetics and electrocatalysis. Structure, microstructure and defect structure serves as the basis for the developing understanding and to evaluate possible use in technologies mentioned above.



Structure and microstructure studies by X-ray diffraction and electron microscopy. Defect concentration and transport properties characterization by thermogravimetry and electrochemical approaches. Surface kinetics/electrocatalysis by the former and in particular use of gaseous isotopes in combination by mass spectroscopy (GPA). All potentially complemented by computational approaches.



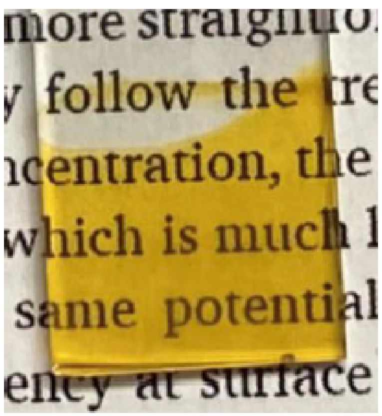
Projects generally consists of a mix of inorganic and physical chemistry and can be designed according to the candidate’s interest. Also joint project with other sections at Chemistry and Physics Department are optional.

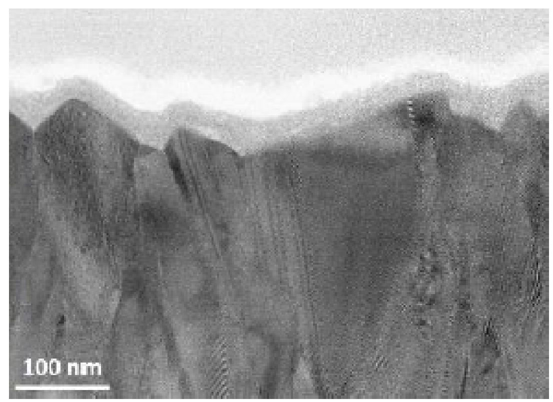
B.Sc. and M.Sc. projects related to photoelectrochemistry (PEC) as part of the Group for Electrochemistry (Headed by Prof. Truls Norby, truls.norby@kjemi.uio.no)

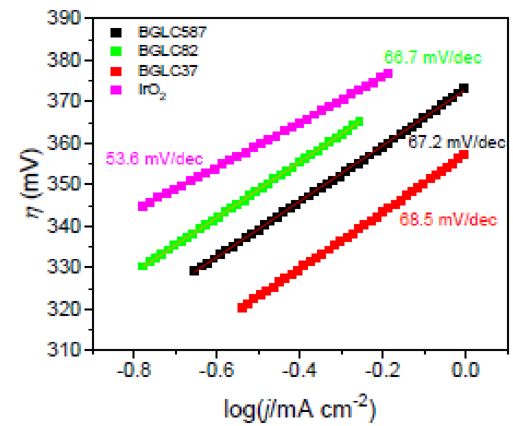
(contact: a.e.chatzitakis@smn.uio.no, A. "Sakis" Chatzitakis)

Main project

1. Tantalum nitride (Ta_3N_5) films on glass and integration in tandem photovoltaic (PV) structures for water electrolysis with solar light. (Kjemi, MENT)

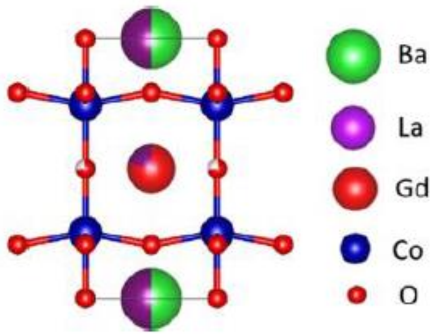


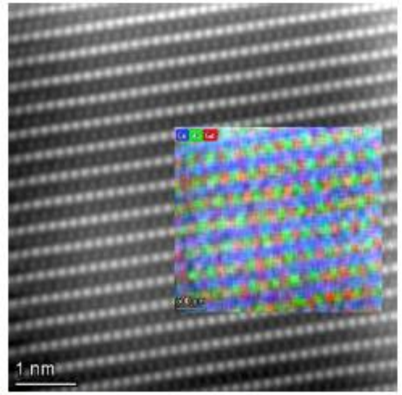


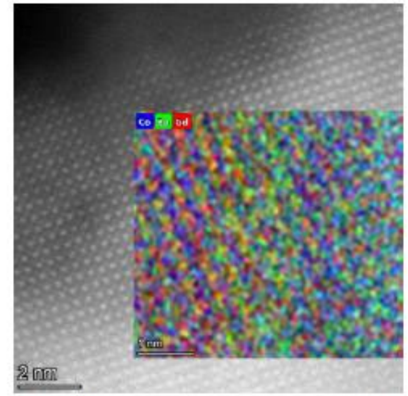


The project will be a traditional photoelectrochemistry one with many parameters to study and look into. A lot of basic electrochemistry and advanced photoelectrochemistry. Synthesis and structural characterisation of thin films of Ta_3N_5 and integrations with PV. Study of the oxygen evolution reaction (OER).

2. Study of the structural evolution of perovskite-based catalysts during water electrolysis. (MENA, Kjemi)



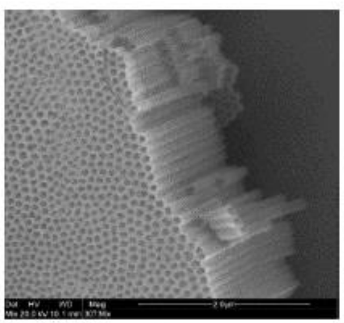


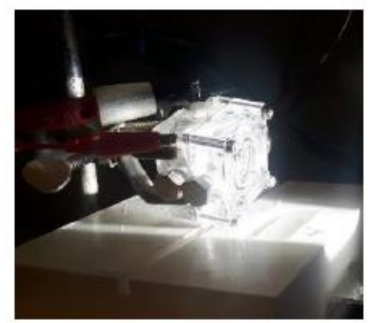


This is a mechanistic study regarding the amorphisation of catalysts during water electrolysis. Advanced synthesis and characterisation methods will be employed for the catalysts and their degradation. This can be coupled with theory and calculations and it will be in collaboration with more from the group.

Complementary project: This can be coupled to project 2 as its application

2.1. Solid state PEC cells for water splitting in the gas phase using catalysts from 2. (MENT, Kjemi)





The project will be a traditional photoelectrochemistry one but our goal is to electrolyse water in the gas phase, i.e. water vapour, with sunlight. Titanium Dioxide (TiO_2) or other nanomaterials modified with catalysts from project 2 will be used for this purpose and the main goal is to connect the gas phase electrolysis cell with a Mass Spectrometer (MS) and detect the production of hydrogen gas, while water vapour is electrolysed.