Programme:

11.00 -	Registration
11.30	Welcome
11.35	Prof. **Kay Severin**: *"Synthetic Chemistry with Laughing Gas"*.
12.20	Lunch (optional)
13.15	Prof. **Jens K. Nørskov**: *"Understanding Transition Metal Heterogeneous Catalysis"*.
14.00	Prof. **Sander Woutersen:** *"New Light on 'Biological' Water and Polyether Solubility"*.
14.45	Coffee break
15.15	Prof. **Bill Morandi**: *"Shuttle Catalysis - a Conceptual Blueprint for Reversible Functional Group Transfer"*.
16.00	Prof. **Torben R. Jensen**: *"Investigations of Hydrides for Energy Storage"*.
16.45	Refreshment
17.00	Project Manager **Dorte Bartnik Johansson**: *"From Idea to Product, from Lignin to a Sustainable Stone Wool Product"*.
18.00	Dinner (optional), Canteen

Local organisers:
Jørgen Skibsted (jskib@chem.au.dk)
Bo Brummerstedt Iversen (bo@chem.au.dk)

Danish Chemical Society

16th Aarhus Winter Meeting

Trends in Modern Chemistry

January 24, 2020

Department of Chemistry
Aarhus University
Langelandsgade 140
DK-8000 Aarhus C.

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Professor **Kay Severin**, Laboratory for Supramolecular Chemistry, École Polytechnique Fédérale de Lausanne (EPFL), Switzerland

Synthetic Chemistry with Laughing Gas
Nitrous oxide (N_2O, 'laughing gas') is rarely used as a reagent in synthetic chemistry. On the contrary, industrially produced N_2O is destroyed by catalytic decomposition into the elements, because release of N_2O is problematic from an environmental point of view. In the lecture, I will show that N_2O can be used as a nitrogen-atom donor for the synthesis of interesting organic molecules such as triazenes, azo dyes, and novel carbene ligands.

Professor **Jens K. Nørskov**, Technical University of Denmark, Kgs. Lyngby, Denmark

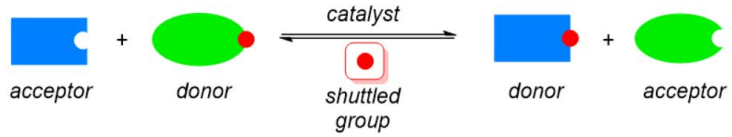
Understanding Transition Metal Heterogeneous Catalysis
The lecture will outline a theory of heterogeneous catalysis that allows a detailed understanding of elementary chemical processes at transition metal surfaces and singles out the most important parameters determining catalytic activity and selectivity. It will be shown how scaling relations allow the identification of descriptors of catalytic activity and how they can be used to construct activity and selectivity maps. The maps can be used to define catalyst design rules and examples of their use will be given.

Professor **Sander Woutersen**, Van't Hoff Institute for Molecular Sciences, University of Amsterdam, the Netherlands

New Light on 'Biological' Water and Polyether Solubility
In the first part of the talk we will have a look at "biological water". Cells are very crowded, and to what extent this affects the properties of intracellular water is heavily debated. Using time-resolved vibrational and dielectric-relaxation spectroscopy we observe the ultrafast random orientational motion of water molecules inside living cells of three prototypical organisms, and investigate how the dynamics of 'biological water' differs from that of tap water. In the second part of the talk, we discuss the solubilities of the two simplest polyethers: PEG (repeating unit $-CH_2-CH_2-O-$), which is present in almost every cosmetic, and POM (repeating unit $-CH_2-O-$), a plastic known to every (former) chemistry student as the brightly-coloured Keck clips for connecting glassware. Surprisingly, PEG dissolves very well in water, but POM is completely insoluble: the opposite of what one might expect from the ratio of hydrophobic to hydrophilic parts in these polymers. Using a combination of experiments and ab-initio MD simulations we try to solve this apparent mystery.

Professor **Bill Morandi**, Department of Chemistry and Applied Bioscience, ETH Zürich. Switzerland

Shuttle Catalysis – a Conceptual Blueprint for Reversible Functional Group Transfer
Catalytic reversible reactions, such as alkene metathesis and transfer hydrogenation, have had an auspicious impact on the molecular sciences. This presentation will describe our efforts to develop related 'shuttle catalysis' reactions for the functionalization and defunctionalization of organic compounds. These reactions avoid the use of toxic reagents (e.g. HCN, CO) through the reversible transfer of chemical moieties between organic molecules. Shuttle catalysis has further been employed in the development of novel C–X (X = S, P) bond metathesis reactions that can help to address significant synthetic challenges across the molecular sciences.



Professor **Torben R. Jensen**, Department of Chemistry, Aarhus University

Investigations of Hydrides for Energy Storage
Hydrogen has an extremely rich chemistry including fascinating structural flexibility and a wide range of compositions and physical properties. A variety of new hydrides have been discovered during the past decade prepared by combined mechano-chemistry and solvent-based methods. These materials are relevant for energy storage as hydrogen in a solid material or as battery materials. Structural dynamics in the solid state, i.e. entropy effects, and structural flexibility created by dihydrogen bonding are of importance for development of new electrolytes.

Project Manager **Dorte Bartnik Johansson**, ROCKWOOL International A/S, Hedehusene, Denmark

From idea to product, from lignin to a sustainable stone wool product
Stone wool products used for insulation, fire protection, growth substrates etc. are based on iorganic stone wool fibers and an organic binder. To increase the sustainability profile of the production, product and the climate, The ROCKWOOL Group is focused on the 17 sustainability goals. One way is to develop new sustainable binders. This start with an idea; such as lignin. Lignin is the second most abundant material in the wool exceeded only by cellulose. But can lignin replace the current petroleum based binder?
The talk will, after introducing the ROCKWOOL Group, focus on development of new products and show the technical challenges and time line from idea to product, from lignin to a sustainable stone wool product.