

Registration:

Online registration is mandatory at:

www.chemsoc.dk

Deadline for registration:

January 13, 2006

Price:

Lectures + coffee: free

Lectures + coffee + lunch: 75,- kr

Lectures + coffee + dinner: 200,- kr

Lectures + coffee + lunch + dinner: 275,- kr

Student discount:

For members of the

Danish Chemical Society:

Lectures + coffee + lunch + dinner: 75,- kr

For non-members:

Lectures + coffee + lunch + dinner: 175,- kr

(student ID required)

To be paid in cash upon arrival

Free transportation from Copenhagen, Odense and Aalborg will be organized for members of the Danish Chemical Society.

Registration at: www.chemsoc.dk

Local organizers:

Jørgen Skibsted

Bo Brummerstedt Iversen

Charlotte Secher

mail: cha@chem.au.dk

phone: 89 42 38 84



Programme:

11:00 Registration, Aud. 6

11:30 Lunch (buffet, optional)

12:30 Welcome

12:35 Professor Sir John M. Thomas

"Benign Methods of Selectively Oxidizing Hydrocarbons: Recent Results"

13:20 Professor Hans W. Spiess

"Elucidating Nanostructures by Nuclear Magnetic Resonance Spectroscopy"

14:05 Professor Peter R. Ogilby

"The Singlet Oxygen Microscope: From Phase-Separated Polymers to a Single Biological Cell"

14:50 Coffee break

15:30 Professor Joachim Sauer

"Structure and Reactivity of Transition Metal Oxides: From Small Gas Phase Species to Nanoclusters and Solid Catalysts"

16:15 Professor Peter E. Nielsen

"Peptide Nucleic Acid (PNA): A Pseudopeptide with Sequence Information. Applications and Implications in Chemistry and Biology"

17:00 Vice president Klaus P. Bøgesø

"Strategies for Improved Antidepressants"

18:15 Dinner (optional) Canteen,

19:30 Beer garden ("fredagsbar", optional)

Danish Chemical Society 2nd Aarhus Winter Meeting

Modern Trends in Chemistry



January 20, 2006

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GRUNDFOS 

 **CHEMINOVA**

 **DANISCO**

First you add knowledge...

**Professor Sir John M. Thomas,
University of Cambridge and Royal
Institution of Great Britain:
“Benign methods of Selectively Oxidizing
Hydrocarbons: Recent Advances”**

In both laboratory and current industrial practice far too much use is made of environmentally aggressive and/or corrosive reagents. Some are used as catalysts: most as stoichiometric oxidants; and many of them are associated with the production of massive quantities of unwanted, harmful or low-grade by-products. By using the strategic principles that emerge from our use of single-site heterogeneous catalysts, it is possible to devise benign methods of selectively oxidizing important commodity chemicals, such as cyclohexane, toluene and the xylenes – using oxygen (largely) or hydrogen peroxide (as well as a solid source thereof) – to yield high-value products under mild conditions.

**Professor Hans W. Spiess,
Max-Planck-Institute for Polymer Research,
Mainz, Germany:
“Elucidating Nanostructures by Nuclear
Magnetic Resonance Spectroscopy”**

In advanced synthetic as well as in biological systems self-assembly of carefully chosen building blocks is crucial for their ability to perform functions such as transport of charge or ions. Such systems, however, are often not crystalline. This renders their structural characterization by conventional scattering methods difficult. High resolution solid state NMR, however, can provide selective structural and dynamic information, requiring only small amounts of as-synthesized samples. Examples elucidating hydrogen bonds and columnar stacking in supramolecular systems as well as self-assembled monolayers are described. The findings are related to specific functions such as photo- or proton conductivity.

**Professor Peter R. Ogilby,
Department of Chemistry, University of Aarhus,
Denmark:
“The Singlet Oxygen Microscope: From Phase-
Separated Polymers to a Single Biological Cell”**

Singlet oxygen, the lowest excited electronic state of molecular oxygen, is an important intermediate in many chemical processes. In complex biological and polymeric systems, the behavior of singlet oxygen can be influenced by microscopic heterogeneities and phase-separated domains. Thus, much can be gained if singlet oxygen is directly monitored with both time and spatial resolution from such systems. We have embarked on a multi-faceted program in which optical spectroscopic techniques are used to create dynamic singlet oxygen images of heterogeneous systems. After a general overview, I will focus on recent experiments on single cells. The results obtained provide a new perspective for mechanistic studies of photoinduced cell death and intracellular signaling which, in turn, have practical applications in Photodynamic Therapy, a medical treatment used to destroy undesired tissue.

**Professor Joachim Sauer,
Institut für Chemie, Humboldt-Universität zu
Berlin, Germany:
“Structure and Reactivity of Transition Metal
Oxides: From Small Gas Phase Species to
Nanoclusters and Solid Catalysts”**

Transition metal oxides in general and vanadium oxides in particular are viable catalysts for the oxidation and oxygenation of hydrocarbons. The mechanisms of the oxidative dehydrogenation of propane and the oxidation of methanol to formaldehyde are examined. Density functional theory (DFT) in concert with experiments is used to answer questions such as: What is the structure of vanadium oxide species when supported on other oxides? What is the structure of gas phase cluster ions and how does it differ from supported species? How does the support affect the reactivity of the active component of a supported catalyst? Can gas phase clusters model the reactivity of solid catalysts?

**Professor Peter E. Nielsen,
The Panum Institute, University of
Copenhagen, Denmark:
“ PNA: A Pseudopeptide with Sequence
Information. Applications and
Implications in Chemistry and Biology”**

PNA (peptide nucleic acid) is a DNA mimic in which the entire backbone has been replaced by a backbone composed of N-(2-aminoethyl)glycine units. PNA is a very good structural mimic of DNA in terms of its ability to form double helical complexes with complementary oligonucleotides or with another sequence complementary PNA. A variety of “folded” PNA structures have also been identified. Finally PNA oligomers (in their native form) are achiral, but chirality may be induced in PNA-double helices. PNA may serve as a model for a non-phosphodiester-ribose based primordial genetic material in the discussion of the origin of life on earth, and is also of potential interest for the discovery and development of novel gene targeted reagents and medical drugs. The lecture will discuss the properties of PNA as a pseudopeptide based information molecule as well as applications in chemistry and biology.

**Vice president Klaus P. Bøgesø,
H. Lundbeck A/S, Denmark:
“Strategies for improved antidepressants”**

The selective serotonin reuptake inhibitors (SSRIs) are the most widely used drugs for the treatment of depressive disorders. The most prominent unmet need of SSRIs is their slow onset of action, i.e. full effect is obtained only after 6-8 weeks of treatment. We have studied a number of SSRI augmentation strategies. For example, addition of concomitant antagonism of certain other serotonin receptors lead to increased serotonin release and faster onset of action. Moreover, an unexpected and highly interesting enhancement effect resulting in faster onset of action and higher efficacy was discovered during the development of the S-enantiomer of citalopram, escitalopram. A recently published crystal structure of a transporter of the same type as the serotonin transporter has allowed an emerging understanding of this effect at the molecular level.