Registration:

Online registration is mandatory at:

www.chemsoc.dk

or by e-mail to

Charlotte Secher: cha@chem.au.dk

Deadline for registration:
January 18, 2008

Price:
Lectures + coffee: free
Lectures + coffee + lunch: 100,- kr
Lectures + coffee + dinner: 200,- kr
Lectures + coffee + lunch + dinner: 300,- kr

Student discount:
For members of the
Danish Chemical Society:
Lectures + coffee + lunch + dinner: 100,- kr

For non-members:
Lectures + coffee + lunch + dinner: 200,- 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,
e-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 Robert Cava
"Superconductive, ferromagnetic, and thermoelectric properties of layered chalcogenides"

13:20 Professor Niels Chr. Nielsen
"NMR studies of fibrils and membrane proteins"

14:05 Coffee break

14:30 Professor Walter Thiel
"Quantum mechanical and molecular mechanical studies of biomolecules"

15:15 Professor Urs Baltensberger
"Atmospheric aerosols – recent developments in elucidating their sources"

16:00 Coffee break

16:20 Professor Jesper Wengel
"Nucleic acid medicinal chemistry – towards new biopharmaceuticals?"

17:05 Research Manager Poul Toft Frederiksen
"Applied chemistry at the heart of the machine industry"

18:00 Dinner (optional) Canteen,

20:00 Beer garden ("fredagsbar", optional)

Danish Chemical Society
4th Aarhus Winter Meeting

Trends in Modern Chemistry

February 1, 2008

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

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First you add knowledge...

Professor Robert J. Cava
Department of Chemistry, Princeton University, NJ, U.S.A.
"Superconductive, ferromagnetic, and thermoelectric properties of layered chalcogenides"

The crystal structures, solid state chemistry, and physical properties of layered chalcogenides have been widely studied, but continue to yield surprises.
This talk will describe our recent observations of the effects of chemical and structural changes on the properties of superconducting early transition metal dichalcogenides, and the thermoelectric properties of the layered bismuth tellurides. We show that the tellurides are a prime example of a layered infinitely adaptive series, and, that when doped with Mn, form a bulk ferromagnetic semiconductor with unexpected defect chemistry.

Professor Niels Chr. Nielsen
Department of Chemistry, University of Aarhus.
"NMR studies of fibrils and membrane proteins"

The presentation will introduce aspects of modern NMR methods for structural analysis of proteins bound to membranes or aggregated into fibril structures.
Besides a brief introduction into technical aspects the focus will be antimicrobial peptides, ion channels, and various peptides/proteins assembling into amyloid fibril structures studied by combinations of liquid- and solid-state NMR spectroscopy, along with biophysical analysis and MD simulations.

Professor Walter Thiel
Max-Planck-Institut für Kohlenforschung, Mülheim an der Ruhr, Germany
"Quantum mechanical and molecular mechanical studies of biomolecules"

In recent years, it has become possible to model chemical reactions in large biomolecules using combined quantum mechanical / molecular mechanical (QM/MM) methods. After a general outline of the theoretical background and the chosen strategy (see Top. Curr. Chem. 2007, 268, 173-290), the lecture will describe some of our recent work on biocatalysis by enzymes, in particular p-hydroxybenzoate hydroxylase (PHBH) and cytochrome P450cam.
In the case of PHBH, the focus will be on methodological advances in QM/MM approaches, while P450cam will serve as an example for the chemical insights that can be provided by QM/MM calculations.
The comparison between the QM/MM results for the enzyme and the QM results for gas-phase model systems allows us to assess the role of the protein environment and to gain an improved mechanistic understanding of enzymatic reactions.

Professor Urs Baltensperger
Laboratory of Atmospheric Chemistry
Paul Scherrer Institut, Villigen, Switzerland
"Atmospheric aerosols – recent developments in elucidating their sources"

Atmospheric aerosols are important because they have adverse health effects and because their impact on climate is still poorly quantified. They are either directly emitted in particulate form into the atmosphere (termed primary particles) or formed from gaseous precursors by atmospheric reactions (secondary particles). Organic aerosols comprise a large fraction of the atmospheric aerosol and the contributions via primary and secondary processes as well as their anthropogenic or biogenic origin are subject of big current debates. This talk will first give an overview of the chemical composition of the atmospheric aerosol and then present insight into recent developments that help elucidating the questions above. The results show that there is a high added value in combining laboratory and field measurements.

Professor Jesper Wengel
Department of Physics and Chemistry, University of Southern Denmark, Odense:
"Nucleic acid medicinal chemistry – towards new biopharmaceuticals?"

Nucleic acids have for several decades promised to deliver solutions to the increasing demands for safer and more efficient drugs against diseases like cancer and viral infections. So far these promises have not been fulfilled. In the lecture I will present an update on the field of therapeutic nucleic acids. Furthermore, with emphasis on LNA (Locked Nucleic Acids), I will discuss how I think that modern nucleic acid chemistry and medicinal chemistry may be the key factor towards realising this class of molecules as the "drugs of the future".

Research Manager Poul Toft Frederiksen
Grundfos, Bjerringbro
"Applied chemistry at the heart of the machine industry"

Building world-class pumps is much more than nuts and bolts. To achieve the required product features such as environmental friendliness lifetime, efficiency and cost, advanced chemistry and materials science is needed: The survival of construction polymers after ten years in hot, aggressive water cannot be ensured by testing just for 1000 hours; for tribology, hard and resistant, yet ductile ceramics are desired; and needed cohesive bonding between metals and plastics, or plastics and rubber will require significant advances in surface chemistry. And water is more than just water: waste water from dairies, fresh ground water for consumption, extremely pure process water, each type possess a new set of chemical challenges for the designer. Moving on to pumping food or chemicals, new vistas of enquiry are opened. Finally, if we want to not only move the liquid, but measure and change its properties, a venerable machine builder may find itself asking serious biochemical questions.
These examples may serve to elucidate the key role of chemistry in one part of the machine industry.