

## Registration:

Online registration is mandatory at:

[www.chemsoc.dk](http://www.chemsoc.dk)

Deadline for registration:

January 14, 2005

## Price:

Lectures + coffee: free

Lectures + coffee + lunch: 75,- kr

Lectures + coffee + dinner: 175,- kr

Lectures + coffee + lunch + dinner: 250,- kr

Student discount:

Lectures + coffee + lunch + dinner: 50,- kr

(student ID required)

## To be paid in cash upon arrival

## Local organizers:

Jørgen Skibsted

Bo Brummerstedt Iversen

Charlotte Secher,

mail: [cha@chem.au.dk](mailto:cha@chem.au.dk)

phone: 89 42 38 84



## Programme:

11:00 Registration, Dept. of Chemistry, aud. 6

12:00 Lunch (optional)  
Canteen, Dept. of Mathematics

13:00 Professor Peter Blaha  
"Physical and structural parameters from  
DFT (Wien2k) calculations"

13:45 Professor Ole G. Mouritsen  
"The physical chemistry of magic bullets"

14:30 Professor Karl Anker Jørgensen  
"Asymmetric catalysis"

15:15 Coffee break

15:45 Professor Krister Holmberg  
"Nanomaterials made from templates  
of self-assembled surfactants"

16:30 Professor Majed Chergui  
"New trends in structural dynamics  
based on ultrashort X-ray pulses"

17:15 Principal Chemist Michael Brorson  
"Heterogeneous catalysis in industry"

18:15 Dinner (optional)  
Canteen, Dept. of Mathematics

19:30 Beer garden ("fredagsbar") (optional)  
Dept. of Chemistry

# Danish Chemical Society Aarhus Winter Meeting

## Modern Trends in Chemistry



January 21<sup>st</sup>, 2005

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

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**Professor Peter Blaha,  
Vienna University of Technology, Austria:  
"Physical and structural parameters from  
DFT (Wien2k) calculations".**

Atomistic first-principles simulations of materials are becoming more and more widely used in modern research work and significantly broaden the knowledge about a specific materials science problem.

The recent advances in this field are due to both, the increased computational power of modern PCs, and the development of sophisticated computer codes, mostly based on density functional theory. I will discuss briefly the features of the widely used WIEN2k package for electronic structure calculations in solids and illustrate it with several examples.

**Professor Ole G. Mouritsen,  
University of Southern Denmark, Denmark:  
"The physical chemistry of magic bullets"**

One of the key problems in the treatment of serious diseases like cancer and inflammation is that many potent drugs are very poisonous and not only kill the deceased cells but also healthy ones.

The term 'magic bullet' was coined by Paul Erlich, the father of modern medicinal chemistry, who in the beginning of the twentieth century envisioned the perfect drug as a 'bullet' that automatically targets and selectively kills the deceased cells without damaging healthy tissue.

Recent research into the physics and physical chemistry of fats (lipids) has suggested that it may be possible to construct nano-scale fat bullets, so-called liposomes that encapsulate and mask potent drugs. The liposomes can effectively invade the human immune system and carry the drug to the target.

By taking advantage of specific biophysical properties of the liposomes on the one side and the peculiar pathophysiological and biochemical properties of e.g. cancer cells on the other side, it is possible in an intelligent way to target the liposomes to the deceased cells and with a particular mechanism, involving certain enzymes, to open the liposomal carriers and unload the drug precisely where the drug is supposed to act.

**Professor Karl Anker Jørgensen,  
University of Aarhus, Denmark :  
"Asymmetric catalysis"**

Chiral molecules are fundamental for all living cells.

In recent years one of the hottest fields in chemistry has been the development of reactions where a chiral molecule, both metal complexes and small organic molecules, catalyze the formation of chiral organic compounds.

The lecture will present some fundamental principles and information in asymmetric catalysis and show the use of organocatalysis for e.g. the formation of chiral drugs which in clinical tests show an improved effect compared to the racemate being on the market.

**Professor Krister Holmberg,  
Chalmers University of Technology, Sweden:  
"Nanomaterials made from templates of  
self-assembled surfactants"**

Surface active molecules, surfactants, self-assemble in water. At low concentration they form micelles and at higher concentration they form liquid crystals with very well-defined geometry.

The liquid crystals may be used as templates for formation of either mesoporous materials, i.e. materials with nano-sized pores extending in one or three directions, or nanorods, which are cylindrical objects.

Mixtures of surfactant, water and oil form micro-emulsions, which may consist of water droplets dispersed in oil and surrounded by a monolayer of surfactant. Such droplets may be used as minireactors for the preparation of inorganic nanoparticles.

Particles in the size range of 3-10 nm can be prepared this way and examples include metals, metal alloys and oxides.

Both the mesoporous materials and the nanoparticles are of considerable interest for catalysis.

**Professor Majed Chergui,  
Ecole Polytechnique  
Federale de Lausanne, Switzerland:  
"New trends in structural dynamics based  
on ultrashort X-ray pulses"**

The advent of femtosecond laser spectroscopy has allowed the possibility to visualize chemical reactions on the time scale of atomic motion.

An increased insight is now made possible with the availability of ultrashort pulses of X-radiation.

We will briefly review the state of the art in ultrafast X-ray diffraction and X-ray absorption (XAS) studies, and will then present our results on ultrafast XAS of coordination chemistry compounds in aqueous solutions.

**Principal Chemist Michael Brorson,  
Haldor Topsøe A/S, Denmark:  
"Heterogeneous catalysis in industry"**

Heterogeneous catalysis forms the basis for both large-scale chemicals production and for environmental protection.

Catalyst discovery and development with the aid of new chemistry and advanced analytical techniques will be exemplified in an industrial context.

Emphasis will be given to catalysts and processes for desulfurization of oil and for removal of NO<sub>x</sub> from exhaust gasses.

Also, the synthesis of new types of materials that may find applications as catalysts will be discussed.