The Danish Chemical Society Annual Meeting 2015

11th of June 2015, Odense
University of Southern Denmark

www.chemsoc.dk
Mission and history of The Danish Chemical Society

The Danish Chemical Society has been founded in 1879 as a society for Danish chemists and has since focused on the advancement of chemistry and the improvement of the public recognition of chemistry. This mission has not changed and is of even more importance today, where modern life is entirely dependent on chemical achievements like materials research (e.g. polymers), and medicinal chemistry (e.g. drug discovery), to name just a few. The public recognition of chemistry needs more young students and researchers in the various branches of chemistry to engage in discussions on important questions in our society. Many global problems are strongly linked to chemistry (e.g. green energy, affordable health care, clean water or the protection of our environment).

Become a member of The Danish Chemical Society and:

- Participate in scientific meetings organized or supported by our society
- Write articles and essays in the society journal – Dansk Kemi
- Apply for travel grants
- Find job offers within the society network
- Receive society awards for outstanding contributions in chemistry (e.g. PhD prizes)
- Organize local meetings for your chemistry division with support from your society
- Promote your career as an invited speaker at our national meetings

Sign up at chemsoc.dk and become a member (1st year of your membership is free)

[annual membership fee - student members: 225 Kr - full members: 450 Kr]

Famous Danish chemists

W. C. Zeise, 1789-1847
New metal-organic compounds (e.g. Zeise’s salt).

J.N. Brønsted, 1879-1947
Key acid-base definition (Brønsted theory).

N. J. Bjerrum, 1879-1958
Theory of strong electrolytes and applied IR spectroscopy.
## Program Agenda

<table>
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<tr>
<th>Time</th>
<th>Event</th>
<th>Room</th>
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<tr>
<td>09.30 – 10.15</td>
<td>Registration</td>
<td>Outside U45</td>
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<tr>
<td>10.15 – 10.20</td>
<td>Welcome</td>
<td>U45</td>
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<tr>
<td>10.20 – 11.30</td>
<td>Plenary lecture by Prof. Dr. A. Stephen Hashmi</td>
<td>U45</td>
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<td></td>
<td>Ruprecht-Karls-Universität Heidelberg, Germany</td>
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<td></td>
<td>“Gold Catalysts, Mechanisms and Synthetic Applications”</td>
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<td>11.30 – 12.45</td>
<td>Lunch and Poster session</td>
<td>&quot;Old Fridaybar&quot;</td>
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<td>12.45 – 14.15</td>
<td>Session lectures I</td>
<td>U46</td>
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<td><em>The Division of Organic Chemistry I</em></td>
<td>U47</td>
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<td><em>The Division of Inorganic Chemistry</em></td>
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<td><em>Danish Society of Molecular Spectroscopy</em></td>
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<td><em>The Danish Society of Analytical Chemistry</em></td>
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<td><em>The Division of Pharmaceutical Chemistry and Technology I</em></td>
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<td><em>Chemical Engineering / IDA Kemi – Kemiingeniørgruppen I</em></td>
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<td><em>The Danish Society of Pharmacology, Toxicology, and Medicinal Chemistry (DSFTM) I</em></td>
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<tr>
<td>14.15 – 14.45</td>
<td>Coffee break</td>
<td>&quot;Old Fridaybar&quot;</td>
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<td>14.45 – 16.15</td>
<td>Session lectures II</td>
<td>U46</td>
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<td><em>The Division of Organic Chemistry II</em></td>
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<td><em>The Danish Society of the History of Chemistry</em></td>
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<td><em>The Division of Theoretical Chemistry</em></td>
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<td><em>The Division of Pharmaceutical Chemistry and Technology II</em></td>
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<td><em>The Danish Society of Pharmacology, Toxicology, and Medicinal Chemistry (DSFTM) II</em></td>
<td>U45</td>
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<tr>
<td>16.20 – 17.00</td>
<td>Bjerrum-Brønsted-Lang award lecture</td>
<td>U45</td>
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<tr>
<td>17.10 – 18.25</td>
<td>Poster session</td>
<td>&quot;Old Fridaybar&quot;</td>
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<td>18.30 – 20.00</td>
<td>Dinner and poster awards</td>
<td>SDU restaurant</td>
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<td>Departure for participants from Copenhagen and Aarhus</td>
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### Session lectures I  
**12.45 – 14.15**

#### The Division of Organic Chemistry / Sektionen for Organisk Kemi

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<tr>
<th>Title</th>
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<th>Time</th>
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<tr>
<td>Development and use of ubiquitin-based reagents</td>
<td>Huib Ovaa</td>
<td>12.45 – 13.25</td>
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<td>Chemical Biology Laboratory, Netherlands Cancer Institute</td>
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<tr>
<td>No need for aromatics. The story about fluorescence in dendrimers</td>
<td>Jørn B. Christensen</td>
<td>13.25 – 13.50</td>
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<td>Department of Chemistry, University of Copenhagen</td>
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<td>Development of the molybdenum-catalyzed deoxydehydration</td>
<td>Peter Fristrup</td>
<td>13.50 – 14.15</td>
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<td>DTU Chemistry, Technical University of Denmark</td>
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#### The Division of Inorganic Chemistry / Sektionen for Uorganisk Kemi

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<tr>
<th>Title</th>
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<tr>
<td>High pressure chemistry and polymorphism of metal oxide perovskites</td>
<td>Martin Bremholm</td>
<td>12.45 – 13.15</td>
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<td>Center for Materials Crystallography, Department of Chemistry, Aarhus University</td>
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<td>Facile synthesis of starch-scaffolded bimetallic Au-Pt nanostructures and their catalytic properties</td>
<td>Christian Engelbrekt</td>
<td>13.15 – 13.45</td>
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<td>NanoChemistry, Department of Chemistry, Technical University of Denmark</td>
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<td>Single crystal EPR measurements on dinuclear chromium(III) complexes</td>
<td>Thorbjørn J. Morsing</td>
<td>13.45 – 14.15</td>
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<td></td>
<td>Department of Chemistry, University of Copenhagen</td>
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### The Danish Society of Molecular Spectroscopy / Dansk Forening for Molekylspektroskopi

**MOLEKYLSPETROSKOPIPRISEN 2015**

**Ultrafast dynamics and time-resolved photoelectron spectroscopy - Experiment, theory, and simulation**  
Thomas Scheby Kuhlman  
The Boston Consulting Group, Copenhagen  

**Characterization of the catalytic cycle of NH$_3$-SCR over copper exchanged chabazite**  
Anita Godiksen  
Centre for Catalysis and Sustainable Chemistry, DTU Chemistry, Technical University of Denmark  

**Direct optical excitation of molecular oxygen in solution and in single mammalian cells**  
Mikkel Bregnhøj  
Center for Oxygen Microscopy, Department of Chemistry, Aarhus University  

### The Division of Analytical Chemistry / Selskabet for Analytisk Kemi

**Two-dimensional liquid chromatography – Optimization of online reversed phase × reversed phase separations**  
Rune Græsbøll  
Department of Plant and Environmental Sciences, University of Copenhagen  

**Ambient ionization techniques for mass spectrometric analysis of compounds on textiles**  
Hans Christian Budtz  
Department of Plant and Environmental Sciences, University of Copenhagen  

**A new research platform in the high Arctic – New research and possibilities within the new research station donated by the Villum foundation**  
Henrik Skov  
Department of Environmental Science, Aarhus University, Roskilde
**The Division of Pharmaceutical Chemistry and Technology/ Sektionen for Farmaceutisk Kemi og Teknologi**

**Effect of autoclaving on the properties of poloxamer-stabilized nanoemulsions**
Judith Kuntsche  
Department of Physics, Chemistry and Pharmacy, University of Southern Denmark

**Saturation and supersaturation measurement of hydrophobic solute with micropipette manipulation technique**
Koji Kinoshita  
Center of Single Particle Science and Engineering, FKF, University of Southern Denmark

**Dissolution rates, supersaturation, nucleation and solubility of NaCl in single water micro droplets into organic liquids**
Anders Utoft  
Center of Single Particle Science and Engineering, FKF, University of Southern Denmark

**IDA Chemistry - Chemical Engineering division / IDA Kemi – Kemiingeniørgruppen**

**Looking inside running batteries - Engineering materials for higher power**
Dorthe Bomholdt Ravnsbæk  
Department of Physics, Chemistry and Pharmacy, University of Southern Denmark

**Forbedret kontrol af selektivitet, polarisation og fouling med dynamiske membransystemer**
Gunnar Eigil Jonsson  
DTU Chemical Engineering, Technical University of Denmark

**Samudrådning af gylle og affald - processen ingen har styr på**
Michael Madsen  
ENVO Group A/S, Aabenraa
The Danish Chemical Society – Annual meeting 2015

Danish Society of Pharmacology, Toxicology and Medicinal Chemistry / Dansk Selskab for Farmakologi, Toksikologi og Medicinalkemi

New Methods for the Synthesis of Isotopically Labeled Pharmaceuticals
Troels Skrydstup
iNANO and Department of Chemistry, University of Aarhus

Targeting protein-protein interactions in the Brain
Kristian Strømgaard
Department of Medicinal Chemistry, University of Copenhagen

Session lectures II

The Division of Organic Chemistry /
Sektionen for Organisk Kemi

Process chemistry: Challenges in chirality and metal catalysis
Mikkel Fog Jacobsen
Lundbeck, Process Research

Synthetic Studies of the Hypoxia-Selective Natural Products Rakicidin A and BE-43547A1
Thomas B. Poulsen
Department of Chemistry, Aarhus University

PhD prize – award lecture
The Danish Society of the History of Chemistry / Dansk Selskab for Historisk Kemi

Kemi i ugeskriftet Ingeniøren før Anden Verdenskrig
Erik Lyngsø-Petersen
Ingeniøren a/s

Hvordan DDT medvirkede til min opdagelse af PCB
Søren Jensen
Department of Environmental Chemistry, University of Stockholm

Indenfor murene: Historier fra fyrværkerifabrikken i Tune
Gry Barfod
Department of Geoscience, University of Aarhus

The Division of Theoretical Chemistry / Sektionen for Teoretisk Kemi

First-principles prediction of interfacial energies – implications for biomineralisation and oil recovery
Martin P. Andersson
Department of Chemistry, University of Copenhagen

Multipole redundancy in Force Field simulations
Sofie Jakobsen
Department of Chemistry, Aarhus University

Electronic energy transfer couplings in heterogeneous environments
Casper Steinmann
Department of Physics, Chemistry and Pharmacy, SDU
IDA Chemistry - Chemical Engineering section /
IDA Kemi – Kemiingeniørgruppen

Design of advanced porous material for catalysis
Jacob Oskar Abildstrøm
CSC Research Centre, DTU Chemistry, Technical University of Denmark

Application of Brønsted acid ionic liquids in Pd-catalyzed ethylene methoxycarbonylation
Eduardo J. Garcia-Suarez
CSC Research Centre, DTU Chemistry, Technical University of Denmark

A consistent reaction cycle for the selective catalytic reduction of nitrogen oxides with ammonia
Susanne Mossin
CSC Research Centre, DTU Chemistry, Technical University of Denmark

The Division of Pharmaceutical Chemistry and Technology /
Sektion for Farmaceutisk Kemi og Teknologi

Super resolution optical microscopy and CARS in human skin applied to transdermal penetration
Jonathan Brewer
Department of Biochemistry and Molecular Biology,
University of Southern Denmark

Investigations on the extrusion process of liposomes by using an instrumented extrusion device
Søren Kristensen
Department of Physics, Chemistry and Pharmacy,
University of Southern Denmark
The Discovery of LEO 29102 - a PDE4 inhibitor for topical treatment of Atopic Dermatitis
Simon Feldbæk Nielsen
LEO Pharma A/S, Ballerup

Drug discovery at Lundbeck, approached to new treatment for brain diseases
Klaus Bæk Simonsen,
Lundbeck A/S, Valby
Plenary lecture Abstract – Prof. Dr. A. Stephen Hashmi

Gold Catalysts, Mechanisms and Synthetic Applications

Homogeneous catalysis by gold has evolved to an important sector of catalysis research.\(^1\) Initially, methodology development clearly dominated, in the last years also an increasing number of applications in synthesis has been reported.\(^2,3\) Efforts to understand the basic mechanism of these reactions continuously accompanied the field.\(^4\)

For twelve years most of the reactions followed simple reaction mechanisms basing on the interaction of one gold centre in a gold complex or organogold compound with the substrate molecule. In most of these reactions vinylgold or alkylgold intermediates are involved, sometimes also gold carbenes.

Now new and interesting principles have been discovered, questions about oxidative addition to gold complexes, propargylic rearrangements, carbene transfer or the lack of β-H-elimination reactions. Furthermore, an entirely new family of reactions, basing on the activation of the organic substrates by two gold complexes at the same time (one π-coordinated, the other σ-coordinated), has been discovered. These open up entirely new synthetic possibilities and follow quite complex mechanisms. These mechanisms, which are new to the whole field of organometallic chemistry, will be discussed in detail.

Some of the new reactions even allow positional selective C,H activations of alkyl side chains, as exemplified below.

The presentation will also contain results from computational chemistry and detailed mechanistic studies including isotope labelling and in situ spectroscopy.

References:

Biographical Information

A. Stephen K. Hashmi received his PhD in 1991 in Chemistry at Ludwig Maximilians University Munich, Germany. He then moved to Stanford University, USA to carry out postdoctoral research on “Enyne metathesis and related reactions (1991-1993) in the group of Prof. B. Trost. He made his Habilitation at the group of Prof. Dr. J. Mulzer during 1993-1998. In 2001 he was appointed Professor for Organic Chemistry at Stuttgart University, Germany. He moved to a chair for Organic Chemistry at Ruprecht-Karls-University Heidelberg, Germany in 2007. He became Dean of the Department of Chemistry in 2010 and since 2013 Vice-Rector of Ruprecht-Karls-University Heidelberg.

He has published around 250 research papers and has received several awards including Heisenberg Fellowship of the Deutsche Forschungsgemeinschaft, Karl-Ziegler Memorial Fellowship, ORCHEM Prize for natural sciences of the German Chemical Society and Hector Research Award.
Bjerrum-Brønsted-Lang award lecture

Prof. Henrik Grum Kjærgaard

Department of Chemistry, University of Copenhagen

“Spectroscopy of Bimolecular Complexes”
University of Southern Denmark (SDU) campus map and conference site
Sponsors

Company Exhibition

Organized by: The Danish Chemical Society / Kemisk Forening

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BioNEC, a centre of Excellence funded by THE VILLUM FOUNDATION for studies on biomolecular nanoscale engineering.