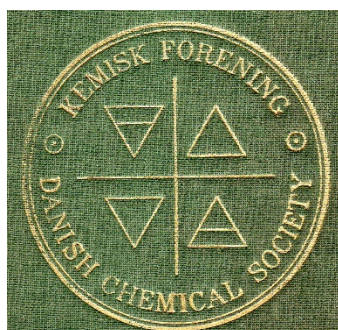


# The Danish Chemical Society Annual Meeting 2019



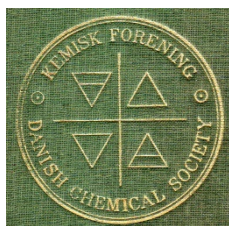
27<sup>th</sup> of June 2019, Copenhagen  
University of Copenhagen

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



KØBENHAVNS  
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## Mission and history of The Danish Chemical Society

The Danish Chemical Society was 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).

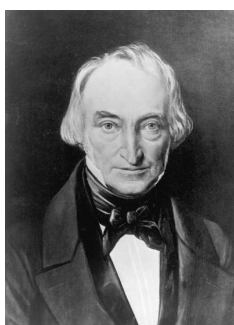
### Become a member of The Danish Chemical Society and:

- ✓ 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](http://chemsoc.dk) and become a member (1<sup>st</sup> year of your membership is free)

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

### Famous Danish chemists



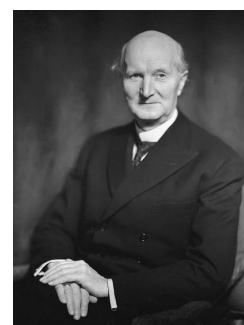
**W. C. Zeise, 1789-1847**

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

### Time

- 10.30 – 11.00**    Registration
- 11.00 – 11.05**    Welcome
- 11.05 – 11.50**    **Plenary lecture by Prof. John C. Warner**  
Warner Babcock Institute for Green Chemistry,  
Wilmington, Mass., USA  
“Green Chemistry: The Missing Elements”
- 11.50 – 12.30**    Lunch and Poster session
- 12.30 – 14.00**    **Session lectures I**  
*The Division of Inorganic Chemistry*  
*The Danish Society for Medicinal Chemistry and Chemical Biology*  
*The Division of Organic Chemistry*  
*The Division of Theoretical Chemistry*
- 14.00 – 14.15**    Coffee break
- 14.15 – 15.45**    **Session lectures II**  
*The Danish Society of Analytical Chemistry*  
*The Danish Society for Medicinal Chemistry and Chemical Biology*  
*The Danish Society of Molecular Spectroscopy*  
*The Division of Pharmaceuticals and Biopharmacy*
- 15.45 – 16.00**    Coffee break
- 16.00 – 17.30**    **Session lectures III**  
*Chemical Engineering / IDA Kemi – Kemiingeniørgruppen*  
*The Division of Organic Chemistry*  
*The Division of Pharmaceuticals and Biopharmacy*
- 17.30 – 18.15**    **Bjerrum-Brønsted-Lang lecture awarded by**  
The Royal Danish Academy of Sciences and Letters
- 18.15 – 19.00**    **Poster session**
- 19.00 –**            Dinner and poster awards
- 20.30**             Departure for participants from Odense and Aarhus

**Session lectures I****12.30 – 14.00****The Division of Inorganic Chemistry /  
Sektionen for Uorganisk Kemi**

**Ultrafast charge carrier dynamics in two-dimensional Ruddlesden-Popper perovskites for stable photovoltaic application** 12.30 – 13.00

Kaibo Zheng

Technical University of Denmark

**Chemistry without bonds - lanthanide coordination chemistry in solution** 13.00 – 13.30

Thomas Just Sørensen

University of Copenhagen

**Beyond graphene: exfoliation and functionalization of magnetic 2D coordination polymers** 13.30 – 14.00

Guillermo Minguez Espallargas

ICMOL, University of Valencia

**The Danish Society for Medicinal Chemistry and Chemical Biology /  
Dansk Selskab for Medicinalkemi og Kemisk Biologi**

**Medchem optimisation of a RORy candidate – working within boundaries.** 12.30 – 13.00

Morten Dahl Sørensen

LEO Pharma, Ballerup, Denmark

**EFMC Candidate Lecture 1** 13.00 – 13.20

Camilla Kaas Frich

Aarhus University

**EFMC Candidate Lecture 2** 13.20 – 13.40

Carlos Moreno-Yruela

University of Copenhagen, Denmark

**EFMC Candidate Lecture 3** 13.40 – 14.00

Raoul Walther

Aarhus University

**Session lectures I****12.30 – 14.00****The Division of Organic Chemistry /  
Sektionen for Organisk Kemi**

**Biosynthetic strategies for development of improved antibody-based drug conjugates for cancer treatment** 10.55 – 11.35

Katrine Qvortrup  
Technical University of Denmark

**Oligomers of indenofluorene-extended tetrathiafulvalenes for conducting materials** 11.35 – 12.00

Line M. Broløs  
Brøndsted Lab, KU SCIENCE, University of Copenhagen

**RNA conjugates with GalNAc as a step towards targeted cholesterol modulation** 12.00 – 12.25

Anders H. Hansen  
Astakhova Lab, Technical University of Denmark

**The Division of Theoretical Chemistry /  
Sektionen for Teoretisk Kemi**

**Operators in Machine Learning: Response Properties in Chemical Space** 12.30 – 13.00

Anders Steen Christensen  
Universität Basel

**Introducing Polarizable Force Fields with non-variational Multipoles: Theory and Implementation for Molecular Dynamics Simulations** 13.00 – 13.30

Pier Paolo Poier  
Aarhus University

**High Throughput Virtual Screening of 230 Billion Molecular Solar Heat Battery Candidates** 13.30 – 14.00

Mads Koertz Madsen  
University of Copenhagen

**Session lectures II****14.15 – 15.45****The Danish Society of Analytical Chemistry /  
Selskabet for Analytisk Kemi**

**Development of analytical tools to investigate conversion of biomass to fuels  
and other products** 14.15 – 14.55

Marianne Glasius  
Institute for Chemistry, Aarhus University

**The Danish Society for Medicinal Chemistry and Chemical Biology /  
Dansk Selskab for Medicinalkemi og Kemisk Biologi**

**Identification of nanomolar inhibitor of RuvBL1/2 from a DNA-encoded small  
molecule library** 14.15 – 14.45

Lars Kolster Petersen  
Vipergen, Copenhagen, Denmark

**NCK Award introduction** 14.45 – 14.50

**NCK Award lecture** 14.50 – 15.40

David Margulies  
Weizmann Institute of Science, Rehovot, Israel

**EFMC Winner announcement** 15.40 – 15.45

Trond Ulven  
University of Copenhagen

**Session lectures II****14.15 – 15.45****The Danish Society of Molecular Spectroscopy /  
Dansk Forening for Molekylspektroskopi**

**Molekylspektroskopiprisen 2019 / The Molecular Spectroscopy Prize 2019** 14.15 – 14.45  
Foredrag af prismodtager / Lecture by prize recipient

**Synthesis of alkali metal water glasses and their characterization by  
multinuclear study of NMR spectroscopy** 14.45 – 15.15  
Sarah Maria Bernadette Wittmann  
Department of Physics, Chemistry and Pharmacy, University of Southern  
Denmark

**Optical Investigation of Single Fluorophores and their Application as Sensitive  
Probes in Soft Matter Science** 15.15 – 15.45  
Stefan Krause  
Nano-Science Center, University of Copenhagen

**The Division of Pharmaceutics and Biopharmacy /  
Sektionen for Farmaci og Biofarmaci**

**From drug substance to drug product: the challenges of peptide instability** 14.15 – 14.45  
Marco van de Weert  
Dept. Pharmacy, University of Copenhagen

**From cells to tissue: the development of keratinocytes into artificial skin** 14.45 – 15.15  
Nicoline Dorothea Jakobsen  
BMB, University of Southern Denmark

**Surface chemistry of pharmaceutical crystals in ethanol-water mixtures** 15.15 – 15.45  
Michael Herzberg  
Dept. Pharmacy, University of Copenhagen

**Session lectures III****16.00 – 17.30****Chemical Engineering / IDA Kemi – Kemiingeniørgruppen****Modified zeolites: synthesis, characterizations and catalytic applications** 16.00 – 16.30

Farnoosh Goodarzi

Centre for Catalysis and Sustainable Chemistry, DTU Chemistry

**Cu-centers in porous catalytic materials studied by in-situ EPR** 16.30 – 17.00

David Nielsen

Centre for Catalysis and Sustainable Chemistry, DTU Chemistry

**Homogenous catalysis for the conversion of biomass to platform chemicals** 17.00 – 17.30

Maria Padilla Paz

Centre for Catalysis and Sustainable Chemistry, DTU Chemistry

**The Division of Pharmaceutics and Biopharmacy /  
Sektionen for Farmaci og Biofarmaci****Impact of the position of phenolic OH-group in tetrahydroxy-phenyl-porphyrins  
on the release and transfer from liposomes** 16.00 – 16.30

Kirishana Rajakulendran

FKF, University of Southern Denmark

**Microwave-induced in situ amorphization** 16.30 – 17.00

Nele Hempel

Dept. Pharmacy, University of Copenhagen

**The Division of Organic Chemistry / Sektionen for Organisk Kemi****PhD prize – award lecture** 16.00 – 16.30**Synthesis of ingenol and beyond – an academia/industry collaboration** 16.30 – 17.00

Lars Jørgensen

LEO Pharma, Ballerup, Denmark

**Recent developments in low pressure carbonylations** 17.00 – 17.30

Troels Skrydstrup

Aarhus University



## Plenary lecture Abstract – Prof. John C. Warner

Warner Babcock Institute for Green Chemistry, LLC  
100 Research Dr., Wilmington, MA 01887, USA  
john.warner@warnerbabcock.com

### Green Chemistry: The Missing Elements

Imagine a world where all segments of society demanded environmentally benign products! Imagine if all consumers, all retailers and all manufacturers insisted on buying and selling only non-toxic materials! The unfortunate reality is that, even if this situation were to occur, our knowledge of materials science and chemistry would allow us to provide only a small fraction of the products and materials that our economy is based upon. The way we learn and teach chemistry and materials science is for the most part void of any information regarding mechanisms of toxicity and environmental harm. Green Chemistry is a philosophy that seeks to reduce or eliminate the use of hazardous materials at the design stage of a materials process. It has been demonstrated that materials and products CAN be designed with negligible impact on human health and the environment while still being economically competitive and successful in the marketplace. This presentation will describe the history and background of Green Chemistry and discuss the opportunities for the next generation of materials designers to create a safer and more sustainable future.



**A farmer spays pesticide on an apple tree in Hanyuan, China** (from “Rethink how Chemical Hazards are Tested” Warner, John C.; Ludwig, Jenifer K. *Nature* 2016, 536 (7616) 269-270).

**John C. Warner**

100 Research Drive  
Wilmington, MA 01887  
978-225-5420

[John@JohnWarner.Org](mailto:John@JohnWarner.Org)  
[www.JohnWarner.Org](http://www.JohnWarner.Org)

John received his BS in Chemistry from UMASS Boston, and his PhD in Chemistry from Princeton University. After working at the Polaroid Corporation for nearly a decade, he then served as tenured full professor at UMASS Boston and Lowell (Chemistry and Plastics Engineering). In 2007 he founded the Warner Babcock Institute for Green Chemistry, with Jim Babcock (a research organization developing green chemistry technologies), and Beyond Benign with Amy Cannon (a non-profit dedicated to sustainability and green chemistry education).

While a senior research group leader at the Polaroid Corporation (1988-1997) Warner coauthored the defining text for the field of Green Chemistry with Paul Anastas and codified the 12 Principles of Green Chemistry. He is the editor of the journal "Green Chemistry Letters and Reviews". Warner is on the advisory panel for the Ellen MacArthur Foundation's New Plastics Economy has been elected a full member of the Club of Rome and is an advisor for Parley for the Oceans where in 2016 he helped create the technology for the Adidas Parley Recycled Ocean Plastics Shoe. He has served as sustainability advisor for several multinational companies. His research and publications in synthetic organic chemistry, noncovalent derivatization, polymer photochemistry and low temperature metal oxide semiconductors has provided the foundation for his theories of what he calls "entropic control in materials design".

The Warner Babcock Institute for Green Chemistry (WBI) is an independent 42,000 sq ft (4000 sq m) research laboratory in Wilmington, Massachusetts fully equipped with state-of-the-art chemistry and engineering equipment. With over 200 patents across more than 70 patent families, he has worked with over 100 fortune 500 companies helping to invent commercially relevant (high performance and appropriate cost) green chemistry technologies across all sectors of the chemical industry. His chemistry inventions have served as the foundation for several new companies, examples include: Collaborative Medicinal Development (ALS Therapy, Phase II Clinical Trials), Hairprint (hair color restoration), Collaborative Aggregates (Delta-S and Delta-Mist, asphalt warm mix, rejuvenator, & spray coat), Lowlight Indoor Solar Energy devices for IoT and BIPV, Formaldehyde and Isocyanate Free wood composite adhesive, and Lithium Cobalt Battery recycling technology.

In 2007 Warner cofounded the nonprofit organization Beyond Benign with Amy Cannon. Collocated at the WBI labs in Wilmington, MA, Beyond Benign creates curricula and training for K-12 and university educators to incorporate concepts of green chemistry and sustainability to improve STEM education. Beyond Benign administers the Green Chemistry Commitment, asking University Chemistry departments to incorporate the principles of green chemistry into their mainstream curricula.

John has received awards as an academic (PAESMEM – President G. W. Bush & NSF, 2004), industrial chemist (Perkin Medal – Society of Chemical Industry, 2014), inventor (Lemelson Ambassadorship – Lemelson Foundation & AAAS) and for governmental chemicals policy (Reinventing Government National Performance Review – Vice President A. Gore & EPA, 1997). He received the American Institute of Chemistry's Northeast Division's Distinguished Chemist of the Year for 2002 and the Council of Science Society President's 2008 Leadership award. Warner was named by ICIS as one of the most influential people impacting the global chemical industries. In 2011 he was elected a Fellow of the American Chemical Society and named one of "25 Visionaries Changing the World" by Utne Reader. He serves as Distinguished Professor of Green Chemistry at Monash University in Australia and in 2017 the German Ministry of Economic Affairs and The Technical University of Berlin announced the naming of "The John Warner Center for Green Chemistry Star-Ups" in his honor.



## Bjerrum – Brønsted – Lang award lecture

**Prof. Leila Lo Leggio**  
Department of Chemistry  
University of Copenhagen

## The Royal Danish Academy of Sciences and Letters



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**Organized by: The Danish Chemical Society / Kemisk Forening**