Thursday, July 11

17:00 Opening ceremony
Room: Margarinfabrikken 1+2+3

17:30 Plenary lectures
Room: Margarinfabrikken 1+2+3
Chair: F. Jensen

18:15 Trygve Helgaker
Esp Høiland — A Pioneer of Computational Quantum Mechanics

19:00 Welcome reception
Room: Margarinfabrikken 1+2+3

Friday, July 12

8:30 Plenary lectures
Room: Margarinfabrikken 1+2+3
Chair: P. Scalise

09:15 Sylvain Canuto
Environment Contribution to Molecular Spectroscopy, Reactivity and Photochemistry

10:30 Sara Ciofﬁni
Modeling Photo-Responsive systems using combined classical and DFT approaches

11:00 Shubhu Li
Generalized energy-based fragmentation approach for large molecules and condensed phase systems

11:30 Pavel Petek
Computational modeling of H+I- migration in porous and layered materials

12:00 Janping Xiao
Towards Computational Design of Catalysts for CO2 Selective Reduction via Reaction Path Diagram Analysis

10:30 Machine learning and data-driven approaches in chemical physics
Room: Margarinfabrikken 2
Chair: A. Aspuru

Multiscale modeling including focused models
Room: Margarinfabrikken 3
Chair: B. Mennucci

Aspect of Heavy-Element Chemistry
Room: Arbeidskontoret
Chair: T. Saue

14:00 Ahmad Mozaffi
Can we derive many-body non-additive polarization energies from 1-body properties and 2-body energies only?

14:30 Krysztof Szalewicz
From molecular properties to intermolecular interaction potentials

15:00 Andreas Haase
Intermolecular interaction energies from fourth order many-body perturbation theory. Impact of individual electron correlation contributions

15:30 Malgorzata M. Szczesniak
New Meta-GGA "Workhorses" in Transition Metal Chemistry and SAPT

16:00 Emergent electronic structure methods
Room: Margarinfabrikken 1+2
Chair: G. Scuseria

Path-integral methods
Room: Margarinfabrikken 3
Chair: F. Pasani

90 years of F12: Hylleraas symposium
Room: Arbeidskontoret
Chair: W. Klopper

17:00 Ali Alavi
Multicomponent Quantum Chemistry: Integrating Electronic and Nuclear Quantum Effects

17:30 Eric Heusken
Variational Excited States in DFT, QMC, and Quantum Chemistry

18:00 Sandeep Sharma
Polynomial scaling multireference methods

18:30 Welcome reception
Room: Margarinfabrikken 1+2+3
**Saturday, July 13**

**Plenary lectures**
Room: Magargiølykke 2-3
Chair: P. Surjan

8:30  
Peter OR  
DMPQ-OS: A new approach to correlation using quadrature

9:15  
Peter Saalfrank  
Molecules driven by light: Electron and nuclear dynamics

**Physico-organic chemistry and catalysis**
Room: Magargiølykke 2-3  
Chair: V. Jensen

10:30  
Robert Paton  
New Mechanisms and Concepts for Organic Reactivity and Reactivity/Selectivity From Computations

11:00  
Kathrin Hagemann  
Is Your Mechanism Correct? Insights into Hydrogenation and Carbonylation Reactions

11:30  
Per-Ola Norby  
Selectivity models for chemical synthesis

12:00  
Benedetta Menucci  
The protein is the key: the unique chemistry of biological pigments revealed by a multiscale strategy

**ERC session**
Room: Magargiølykke 2

12:45-13:45  
Danielle Mammoli (ERC)  
European Research Council session

13:45-14:45  
35 years of 122: Hylleraas symposium  
Room: Magargiølykke 2  
Chair: T. Helgaker

14:00  
Angela Wilson  
Resolution-of-the-identity and Beyond

14:30  
Florian Bischoff  
Explicitly Correlated Coupled-Cluster in Real Space

15:00  
Andreas Grünzke  
Recent progress in applying periodic coupled cluster theory to solids and surfaces

15:30  
Andreas Kühn  
Computing molecular properties in multireference coupled-cluster theory

16:00  
Aurora Clerk  
Heavy Elements Solution Chemistry – A Squeeze Through Ideal and Non-Ideal Solutions and Their Interfaces

17:00  
Jochen Kolb/Bach  
Chemical bonding, core spectroscopy, and magnetic properties of actinide complexes

17:30  
Kwang Li  
Spin-Orient symmetry Breaking and Restoring in Kramer’s-Unrestricted Multireference Approaches

18:00  
Michael Reppy  
All-electron relativistic four-component Dirac-Kohn-Sham theory for solids using Gaussian-type functions

19:00  
Poster session 1

**Posters 1-4:** On the walls outside Magargiølykke 2-3  
**Posters 25-42:** In the meeting room Postnarost  
**Posters 59-74:** In the meeting room Kjærantskontoret

**Sunday, July 14**

**Plenary lectures**
Room: Arbeidskontoret 2-3  
Chair: P. Oral

8:30  
Sara Fernandez  
Prediction of Intramolecular Reorganization Energy Using Machine Learning

9:30  
Thomas Høine  
Challenges for automated materials discovery

9:30  
Alan Apsru-Guill  
The Materials for Tomorrow, Today

**Machine learning and data-driven approaches in chemical physics**
Room: Magargiølykke 2-3  
Chair: G. Chalasinski

**Molecular properties and interactions**
Room: Magargiølykke 2-3  
Chair: D. Wilson

9:00  
Alexandre Gutsche  
Towards Exact Molecular Dynamics Simulations with Quantum Chemistry and Machine Learning

9:30  
Benedetta Menucci  
The protein is the key: the unique chemistry of biological pigments revealed by a multiscale strategy

**ERC session**
Room: Arbeidskontoret 2-3

9:45-10:45  
Danielle Mammoli (ERC)  
European Research Council session

10:45-11:45  
35 years of 122: Hylleraas symposium  
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19:00  
Poster session 2

**Posters 5-24:** On the walls outside Magargiølykke 2-3  
**Posters 25-58:** In the meeting room Postnarost  
**Posters 59-74:** In the meeting room Kjærantskontoret  
**Posters 75-138:** In the room Arbeidskontoret 2-3
Sunday, July 14

Computational spectroscopy: from X-rays to microwaves
Room: Mørgenfjbækken 1+2
Chair: T. Markland

10:30
Shud Mukamel
Ultrafast spectroscopy and imaging of molecules with classical, quantum, and many-body physics
Anna-Sophia Hein

11:00
Maïmora Beziyko
From spectroscopic signatures to 3-D structure of protein building blocks
Mariana Ross

11:30
Jonathan Tennyson
The ExoMol project: molecular line lists for the opacity of exoplanets and other hot atmospheres
Jonathan Tennyson

12:00
Elke Faulkner
Time-Resolved Measurement of Interparticle Coulombic Decay Processes
Francesco Piscini

Monday, July 15

Plenary lectures
Room: Mørgenfjbækken 1+2+3
Chair: K. Brøn

8:30
Thomas F. Miller
Classical and Machine-Learning Methods for Quantum Simulation

9:15
Irene Burghardt
High-Dimensional Quantum Dynamics of Functional Organic Polymer Materials: Coherence, Confinement, and Disorder

10:30
Victor Ruzzo
Accurate, Scalable All-Electron Theory Across the Periodic Table: Organic, Inorganic, Hybrid
Brenda Rubenstein

11:00
Christian Ohserfeld
Quantum-chemical methods for biochemical systems
Ingo Ehrlich

11:30
Joost VandeVende
Linear scaling DFT accelerated with GPUs and ML
Takasi Kanai

12:00
Stevan G. Lončar
Many-electron Correlations in Multi-particle Excitations and Nonlinear Optical Processes in Materials
Tatjana Korneva

14:00
Sascha Rojahn
From picoseconds to attoseconds: Nuclear and electron dynamics
Sascha Rojahn

14:30
Natalie Fey
Calculating calculation before experiment in organometallic catalysis
Eberhard Gross

15:00
Markus Reiter
Quantum Chemical Exploration of Catalytic Reaction Networks
Monika Fuxreiter

16:30
Heather J. Kukl
Transition metal catalyst discovery with high-throughput screening and machine learning
Southera Farimani

17:00
Tucker Carrington
Computational methods for computing vibrational spectra
Seungjo Jung

17:30
Ad van der Avoird
Spectra of O2 induced by collisions with N2 and O2
Philippe Corps

18:00
Fabien Gatti
The polyelectrolyte approach: recent applications to spectroscopy
On Lage

18:00
Poster session 2

Posters 21-30: On the walls outside Mørgenfjbækken 1+2+3
Posters 25-42: In the meeting room Prostneset
Posters 25-74: In the meeting room Importkontoret
Posters 25-10: In the room Importkontoret 1+2
Posters 25-138: In the room Importkontoret 1+2
Tuesday, July 16

8:30
Guilte Gahl
Simulating energy conversion processes from first principles
Chair: D. Crawford

9:15
Zhigang Shui
Density matrix renormalization group: time-dependent folding, light-emitting, carrier transport, and single spin fusion
Room: Møgarefabrikken 2
Chair: O. Brändas

9:45
Yunqiang Jiao
Catalysts Discovery and Understanding with Computational and Data-Driven Approaches
Trist A. Duarte
Unveiling the chemical reactivity of sulfide mineral surfaces in the presence of water and oxygen
Pavel Jurelle
Calculations of three body recombination and dimer product distributions from ultrasonic atomic collisions
Sidney J. Bartlett
The devil’s triangle in XS-DFT calculations and how to fix it
Room: Møgarefabrikken 1
Chair: E. Brändas

10:15
Carine Michel
Understanding reactivity at the catalyst/liquid interface
Johannes Neugebauer
Exact Subsystem Time-Dependent Density-Functional Theory
John Bohn
Ultracold Collisions of Polyatomic CdSbMolecules
Alia Tadjer
Molecular modelling of hybrid ion batteries
Room: Møgarefabrikken 1
Chair: A. Csaszar

11:00
Ian Loin
Simulations of Ion Solvation and Transfer by Adaptive-Partitioning QM/MM Dynamics
Marcus Ellner
Multi-scale methods for electron and excion transfer in biological and organics
Robin Cole
Optical production of polyatomic complex in ultracold regime
Martin Quack
Fundamental and approximate symmetries, parity violation and tunnelling in chiral and achiral molecules
Room: Møgarefabrikken 3
Chair: M. Mayes

11:45
Michelle Coots
Catalysing and Controlling Chemical Reactions with Electric Fields
Tyusho Mihashi
Linear-sitting DFT simulations of complex nano-structured materials using the CONQUEST code
Tipp Karman
Cofacial loss of ultracold molecules
Clémentsr Nicolas
Attoscand-resolved Quantum Chemistry. Predictions from the early years and comparison with recent experiments
Room: Møgarefabrikken 3
Chair: B. Brandal

12:30
Emergent electronic structure methods
Room: Møgarefabrikken 2
Chair: J. Hättig
Computational spectroscopy: from X-rays to microwaves
Room: Møgarefabrikken 2
Chair: V. Liegeois
Computational biophysics
Room: Møgarefabrikken 2
Chair: R. Juliere

13:15
Michael van Setten
Benchmarking GW for quantum chemistry applications
Yannis Galimathas
X-ray Ramam scattering of liquids
Inaki Turon
Quantum Hydride Transfer in Formate Dehydrogenase: Environment Reorganisation and Primary and Secondary Hydrogen Motions
Room: Møgarefabrikken 3
Chair: O. Eisenstein

13:45
Stefan Goedeecker
Wavelets for electronic structure calculations, an introduction and overview
Vincenzo Genova
Quantum solutions: a look at the surface
Marta Jeen Raimo
Understanding enzymatic reactions
Room: Møgarefabrikken 3
Chair: J. Hutson

14:30
Luigi Genovese
Potentialities of Wavelet formalisms for large-scale DFT calculations and beyond
Barbara Brenna
Calculation of X-Ray Absorption and Photoemission Spectra of Molecules in Complex Environment
Qing Cai
QM/MM analysis of metalloenzymes: developments and applications
Fernanda Duarte Gonzalez
Unraveling the Role of Non-Covalent Interactions in Recognition and Catalysis
Room: Møgarefabrikken 3
Chair: J. Hutson

15:00
Large-scale electronic structure models of materials
Room: Møgarefabrikken 2
Chair: H. Håk
From picoseconds to attoseconds: Nuclear and electron dynamics
Room: Møgarefabrikken 2
Chair: F. Martin
Ultracold chemical physics
Room: Møgarefabrikken 3
Chair: P. Juliere

15:45
Woo Yoon Kim
Efficient hybrid density functional calculations in real-space numerical grid methods
David Clary
Quantum Tunneling in Chemical Reactions
Rosario Gonzalez-Ferez
Rydberg polaronic molecules: Electronic structure and experimental proposal for their creation
Room: Møgarefabrikken 3
Chair: F. Martin

16:15
Beatriz Gonzalez del Rio
Large-scale Ab Initio Simulations with Orbital-free Density Functional Theory
Francois Gourdon
Spatial and temporal localization of the vibrational and photoelectron wave packets in LiH photoisomerized by intense free-cycle light pulses
Timur Tcherbul
Magnetic tuning of ultracold chemical reactions: Theoretical insights
Room: Møgarefabrikken 3
Chair: A. Bende

16:45
Quantum Maran
Multi-scale approach: a versatile platform for investigating novel two-dimensional material-based device concepts
Ulla Smirnova
Synthetic chiral light for extremely efficient laser chiral discrimination
Christiane Koch
Quantum effects in cold and controlled molecular dynamics
Room: Møgarefabrikken 3
Chair: A. Bende

17:30
David Tomanek
Magic with Semiconductor 2D Nanomaterials
Morgane Vacher
Insights into chiral luminescence from molecular dynamics simulations and machine learning analysis
Gudrun Quirmener
Shielding ultracold molecules against losses in collision
Room: Møgarefabrikken 3
Chair: J. Hutson

18:30
Conference dinner
Room: Margarinfabrikken 1+2+3

Wednesday, July 17

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