Thursday, July 11

17:00	**Opening ceremony** *Room: Margarinfabrikken 1+2+3*
	Plenary lectures *Room: Margarinfabrikken 1+2+3* **Chair: F. Jensen**
17:30	**Sharon Hammes-Schiffer** *Multicomponent Quantum Chemistry: Integrating Electronic and Nuclear Quantum Effects*
18:15	**Trygve Helgaker** *Egil Hylleraas — A Pioneer of Computational Quantum Mechanics*
19:00	**Welcome reception** *Room: Margarinfabrikken 1+2+3*

Friday, July 12	**Plenary lectures** *Room: Margarinfabrikken 1+2+3* **Chair: P. Szalay**
8:30	**Peter Schwerdtfeger** *The Year of the Periodic Table - Going Superheavy*
9:15	**Sylvio Canuto** *Environment Contribution to Molecular Spectroscopy, Reactivity and Photochemistry*

	Large-scale electronic structure models of materials *Room: Margarinfabrikken 1* **Chair: T. Heine**	**Machine learning and data-driven approaches in chemical physics** *Room: Margarinfabrikken 2* **Chair: A. Aspuru-Guzik**	**Multiscale modeling including focussed models** *Room: Margarinfabrikken 3* **Chair: B. Mennucci**	**Aspect of Heavy-Element Chemistry** *Room: Arbeidskontoret* **Chair: T. Saue**
10:30	**Ilaria Ciofini** *Modeling Photo-Responsive systems using combined classical and DFT approaches*	**Pavlo Dral** *Quantum Chemistry Assisted by Machine Learning*	**Oleg Prezhdo** *Time-Domain Modeling of Excited State Dynamics in Halide Perovskites*	**Thomas Albrecht-Schmitt** *An Unexpected Route to the Formation of Covalent Bonds in Cerium and Berkelium Coordination Complexes*
11:00	**Shuhua Li** *Generalized energy-based fragmentation approach for large molecules and condensed phase systems*	**Cecilia Clementi** *Machine Learning Models for Biomolecular Dynamics*	**Damien Laage** *Water at electrified graphene interfaces: structure, dynamics, vibrational SFG spectroscopy and consequences for electron transfer reactions*	**Katharina Boguslawski** *Simplified Coupled Cluster Methods for f0 Actinide Compounds*
11:30	**Petko Petkov** *Computational modeling of H/H+ migration in porous and layered materials*	**Marivi Fernandez-Serra** *Machine learning a highly accurate exchange and correlation functional of the electronic density*	**Dominika Zgid** *Finite temperature Green's function theories for periodic systems*	**Han-Shi Hu** *Bonding Pattern Change Induced by Relativistic Effects*
12:00	**Jianping Xiao** *Toward Computational Design of Catalysts for CO2 Selective Reduction via Reaction Phase Diagram Analysis*	**Koji Tsuda** *Expanding the horizon of automated metamaterials discovery via quantum annealing*	**Thomas Markland** *Accurate and Efficient Non-adiabatic Quantum Dynamics using Master Equations*	**Michael Patzschke** *Combined computational and spectroscopical analysis of tetravalent f-element complexes*
	Molecular properties and interactions *Room: Margarinfabrikken 1+2* **Chair: A. Rizzo**	**Multiscale modeling including focussed models** *Room: Margarinfabrikken 3* **Chair: S. Höfener**	**Aspect of Heavy-Element Chemistry** *Room: Arbeidskontoret* **Chair: R. Berger**	
14:00	**Alston Misquitta** *Can we derive many-body non-additive polarization energies from 1-body properties and 2-body energies only?*	**Filippo Lipparini** *A general linear scaling implementation for polarizable embedding methods*	**Luuk Visscher** *Relativistic coupled cluster for a new generation of supercomputers*	
14:30	**Krzystof Szalewicz** *From molecular properties to intermolecular interaction potentials*	**Jean-Philip Piquemal** *Scalable polarizable molecular dynamics using Tinker-HP*	**Andre Severo Pereira Gomes** *Relativistic equation of motion coupled cluster based on four-compoment Hamiltonians*	
15:00	**Andreas Hesselmann** *Intermolecular interaction energies from fourth order many-body perturbation theory. Impact of individual electron correlation contributions*	**Debashree Ghosh** *Photo-processes in biological systems – Need for hybrid QM/MM with polarization*	**Hiromi Nakai** *Relativistic density functional theory with picture-change corrected electron density*	
15:30	**Malgorzata M. Szczesniak** *New Meta-GGA "Workhorses" in Transition Metal Chemistry and SAPT*	**Ksenia Bravaya** *Simulating Electron Transfer in Biomolecules: the Role of Polarization and Long-range Electrostatic Interactions*	**Florian Weigend** *NMR Shielding Tensors and Shifts in the Local Exact Two-Component Theory*	
	Emergent electronic structure methods *Room: Margarinfabrikken 1+2* **Chair: G. Scuseria**	**Path-integral methods** *Room: Margarinfabrikken 3* **Chair: F. Paesani**	**90 years of r12: Hylleraas symposium** *Room: Arbeidskontoret* **Chair: W. Klopper**	
16:30	**Ali Alavi** *Non-unitary Quantum Chemistry*	**David Ceperley** *Melting of the 2D Wigner Crystal*	**Edit Matyus** *Ultra-precise computations for molecular paradigms*	
17:00	**Cyrus Umrigar** *Semistochastic Heatbath Configuration Interaction Method and Orbital Optimization*	**Mark Tuckerman** *A path-integral sampling (trajectory-free) approach to the calculation of quantum time correlation functions*	**Kirk Peterson** *On the Development of Accurate Gaussian Basis Sets for f-Block Elements - Initial Efforts for F12 Correlation Consistent Basis Sets for Uranium*	
17:30	**Eric Neuscamman** *Variational Excited States in DFT, QMC, and Quantum Chemistry*	**Jian Liu** *Path integral Liouville dynamics & a unified framework for path integral molecular dynamics*	**David Tew** *Principal Domains in Local Correlation Theory*	
18:00	**Sandeep Sharma** *Polynomial scaling multireference methods*	**Nancy Makri** *Modular Quantum and Rigorous Quantum-Classical Real-Time Path Integral Methods*	**Hans-Joachim Werner** *Explicitly correlated local coupled-cluster methods for large molecules*	

Saturday, July 13	**Plenary lectures** *Room: Margarinfabrikken 1+2+3* **Chair: P. Surjan**			
8:30	**Peter Gill** *Q-MP2-OS: A new approach to correlation using quadrature*			
9:15	**Peter Saalfrank** *Molecules driven by light: Electron and nuclear dynamics*			
	Physical organic chemistry and catalysis *Room: Margarinfabrikken 1* **Chair: V. Jensen**	**Machine learning and data-driven approaches in chemical physics** *Room: Margarinfabrikken 2* **Chair: C. Clementi**	**From picoseconds to attoseconds: Nuclear and electron dynamics** *Room: Margarinfabrikken 3* **Chair: D. Clary**	**Aspect of Heavy-Element Chemistry** *Room: Arbeidskontoret* **Chair: W. Liu**
10:30	**Robert Paton** *New Mechanisms and Concepts for Organic Reactivity and Enantioselectivity From Computations*	**Olexandr Isayev** *Neural networks learning quantum chemistry*	**Todd J. Martinez** *Potential Energy Surfaces and Nonadiabatic Dynamics in Photoactive Proteins from First Principles*	**Stefaan Cottenier** *Po-containing molecules in fission and fusion reactors*
11:00	**Kathrin Hopmann** *Is Your Mechanism Correct? Insights into Hydrogenation and Carboxylation Reactions*	**Johannes Hachmann** *A Machine Learning Shortcut to Physics-Based Modeling and Simulations*	**Regina de Vivie-Riedle** *Photostability of Uracil affected by RNA environment or shaped light*	**Helene Bolvin** *Magnetic coupling between f centers from first principles*
11:30	**Per-Ola Norrby** *Selectivity models for chemical synthesis*	**Alexandre Tkatchenko** *Towards Exact Molecular Dynamics Simulations with Quantum Chemistry and Machine Learning*	**Leticia Gonzalez** *Excited state dynamics of transition metal complexes using efficient trajectory surface hopping methods*	**Juha Vaara** *Computations of Small Physical Effects in Nuclear Magnetic Resonance*
12:00	**Benedetta Mennucci** *The protein is the key: the unique chemistry of biological pigments revealed by a multiscale strategy*	**Volker Deringer** *From Machine-Learning Interatomic Potentials to Atomic-Scale Materials Science*	**Graham Worth** *Simulating Non-adiabatic Photochemistry using Grids and Gaussians*	**Michal Jaszunski** *Nuclear magnetic dipole moments from NMR experiments*
	ERC session *Room: Margarinfabrikken 2*			
12:45-13:45	**Daniele Mammoli (ERC)** *European Research Council session*			
	90 years of r12: Hylleraas symposium *Room: Margarinfabrikken 1* **Chair: T. Helgaker**	**Molecular properties and interactions** *Room: Margarinfabrikken 2* **Chair: D. Wilson**	**Path-integral methods** *Room: Margarinfabrikken 3* **Chair: T. Miller**	
14:00	**Angela Wilson** *Resolution-of-the-Identity and Beyond*	**Katharine Hunt** *New ab initio results for interaction-induced dipoles and susceptibilities and new analytical results for transition probabilities*	**Stuart Althorpe** *Real-time dynamics from imaginary-time path-integrals: theory and practice*	
14:30	**Florian Bischoff** *Explicitly Correlated Coupled-Cluster in Real Space*	**Jacob Kongsted** *Polarizable Density Embedding for Proteins: Excited States in Complex Environments*	**David Manolopoulos** *Path integral methods for reaction rates*	
15:00	**Andreas Grüneis** *Recent progress in applying periodic coupled cluster theory to solids and surfaces*	**Toon Verstraelen** *Modeling Weak Interactions With Spherical Atomic Electron Densities*	**Joseph Lawrence** *On the calculation of quantum mechanical electron transfer rates*	
15:30	**Andreas Köhn** *Computing molecular properties in multireference coupled-cluster theory*	**Denis Jacquemin** *Searching for Super-Accuracy in Excited State Calculations*	**Jeremy Richardson** *Nonadiabatic quantum transition-state theory*	
	Aspect of Heavy-Element Chemistry *Room: Margarinfabrikken 1* **Chair: P. Pyykkö**	**Emergent electronic structure methods** *Room: Margarinfabrikken 2* **Chair: A. Szabados**	**Multiscale modeling including focussed models** *Room: Margarinfabrikken 3* **Chair: L. Slipchenko**	
16:30	**Aurora Clark** *Heavy Element Solution Chemistry – A Sojourn Through Ideal and Non-Ideal Solutions and Their Interfaces*	**Piotr Piecuch** *Toward Exact Quantum Chemistry by a Combination of Stochastic Wave Function Sampling and Deterministic Coupled-Cluster Computations*	**Aurelien de la Lande** *Toward First Principles Simulations of Biological Matter under Ionizing Radiations*	
17:00	**Jochen Autschbach** *Chemical bonding, core spectroscopy, and magnetic properties of actinide complexes*	**Gustavo Scuseria** *Quantum Chemistry for Strong Correlation*	**Joachim Sauer** *Ab initio Free Energy Calculations with Chemical Accuracy for Molecule - Surface Interactions*	
17:30	**Xiaosong Li** *Spin-Orbit Symmetry Breaking and Restoring in Kramers-Unrestricted Multireference Approaches*	**Paola Gori-Giorgi** *Strong-coupling limit in DFT and Hartree-Fock: kinetic correlation energy and dispersion*	**Chao-Ping Hsu** *Machine learning for electron-transfer couplings*	
18:00	**Michal Repisky** *All-electron relativistic four-component Dirac–Kohn–Sham theory for solids using Gaussian-type functions*	**Laura Gagliardi** *Multireference Methods for Extended Systems*	**Rosa Bulo** *Multi-scale Modeling of Chemistry in Water*	
19:00	**Poster session 1**			
	Posters 1-14: On the walls outside *Margarinfabrikken 1+2+3*	**Posters 25-42:** In the meeting room *Prostneset*	**Posters 59-74:** In the meeting room *Kjøpmannskontoret*	
	Posters 15-24: On the walls of the meeting room *Skarven*	**Posters 43-58:** In the meeting room *Importkompaniet*	**Posters 75-139:** In the room *Arbeidskontoret 1+2*	

Sunday, July 14	**Machine learning and data-driven approaches in chemical physics** *Room: Margarinfabrikken 1+2* **Chair: P. Dral**	**Molecular properties and interactions** *Room: Margarinfabrikken 3* **Chair: G. Chalasinski**	**Computational biophysics** *Room: Arbeidskontoret* **Chair: M. Ramos**
8:30	**Şule Atahan-Evrenk** *Prediction of Intramolecular Reorganization Energy Using Machine Learning*	**Berta Fernandez** *Pursuing accuracy in intermolecular potentials and spectra*	**Helmut Grubmüller** *Atomistic Simulation of Biomolecular Function: Ribosomal Translation, Ligand Binding Heterogeneity, and a Dynasome Perspective*
9:00	**Thomas Heine** *Challenges for automated materials discovery*	**Patrick Norman** *VeloxChem: an efficient implementation of real and complex response functions at the level of Kohn–Sham density functional theory*	**Nathalie Reuter** *Interfacial choline-aromatic cation-pi interactions can contribute as much to peripheral protein affinity for membranes as aromatics inserted below the phosphates*
9:30	**Alan Aspuru-Guzik** *The Materials for Tomorrow, Today*	**Sonia Coriani** *Molecular Properties and Interactions: A Wonderful Playground for a Theoretical Chemist*	**Teresa Head-Gordon** *How to Make an Enzyme: Computational Optimization of Electric Fields for Better Catalysis Design*

Sunday, July 14	**Computational spectroscopy: from X-rays to microwaves** *Room: Margarinfabrikken 1+2* **Chair: H. Ågren**	**Path-integral methods** *Room: Margarinfabrikken 3* **Chair: T. Markland**	**90 years of r12: Hylleraas symposium** *Room: Arbeidskontoret* **Chair: M. Hoffman**
10:30	**Shaul Mukamel** *Ultrafast spectroscopy and imaging of molecules with classical, quantum, and noisy x-ray pulses*	**Angelos Michaelides** *Towards an improved understanding of interfacial water*	**Anna-Sophia Hehn** *Explicitly correlated wave function approaches based on the random phase approximation*
11:00	**Malgorzata Biczysko** *From spectroscopic signatures to 3-D structure of protein building blocks*	**Mariana Rossi** *Anharmonic Nuclear Quantum Effects and their Interplay with the Electronic Structure of Weakly Bonded Systems*	**Seiichiro L. Ten-no** *Explicitly correlated F12 theory on modern electronic structure calculations*
11:30	**Jonathan Tennyson** *The ExoMol project: molecular line lists for the opacity of exoplanets and other hot atmospheres*	**Michele Ceriotti** *Efficient Modeling of Thermal and Quantum Fluctuations in Materials and Molecules*	**Jan M. L. Martin** *Do CCSD and Approximate CCSD-F12 Variants Converge to the Same Basis Set Limits? The Case of Atomization Energies*
12:00	**Elke Fasshauer** *Time-Resolved Measurement of Interparticle Coulombic Decay Processes*	**Francesco Paesani** *Nuclear Quantum Effects in Ion-Mediated Hydrogen-Bond Rearrangements*	**Ludwik Adamowicz** *Quantum-mechanical non-Born-Oppenheimer calculations of small atoms and molecules*

Monday, July 15	**Plenary lectures** *Room: Margarinfabrikken 1+2+3* **Chair: R. Broer**
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*

	Large-scale electronic structure models of materials *Room: Margarinfabrikken 1* **Chair: D. Fedorov**	**Emergent electronic structure methods** *Room: Margarinfabrikken 2* **Chair: J. Pittner**	**Molecular properties and interactions** *Room: Margarinfabrikken 3* **Chair: K. Szalewicz**	**Computational biophysics** *Room: Arbeidskontoret* **Chair: P. Imhof**
10:30	**Volker Blum** *Accurate, Scalable All-Electron Theory Across the Periodic Table: Organics, Inorganics, Hybrids*	**Claudia Filippi** *The force awakens in quantum Monte Carlo*	**Stefan Grimme** *New Tight-Binding Quantum Chemistry Methods for the Exploration of Chemical Space*	**Madhurima Jana** *Stability of Proteins in Solutions: A Microscopic Investigation on the Role of Surrounding Water/Cosolvent*
11:00	**Christian Ochsenfeld** *Quantum-chemical methods for biochemical systems*	**Brenda Rubenstein** *Ab Initio Finite Temperature Auxiliary Field Quantum Monte Carlo for Solids*	**Lyudmila Slipchenko** *Polarizable embedding for biological systems: Modeling photoactive proteins with the Effective Fragment Potential method*	**Michele Cascella** *Simulating Biological Systems Coupling Particles and Fields with Molecular Dynamics*
11:30	**Joost VandeVondele** *Linear scaling DFT accelerated with GPUs and ML*	**Fabien Bruneval** *The linearized GW density matrix*	**Attila Csaszar** *Quasistructural molecules*	**Mikko Karttunen** *Computational modelling of cellulose and its modifications*
12:00	**Steven G. Louie** *Many-electron Correlations in Multi-particle Excitations and Nonlinear Optical Processes in Materials*	**Katarzyna Pernal** *Dynamic Correlation for CASSCF Reference with Adiabatic Connection Approaches: Open Shell Systems and Dispersion Interaction*	**Tatiana Korona** *On the Applicability of Various Partitioning Schemes to Intermolecular Interactions*	**Monika Fuxreiter** *Conformational heterogeneity in enzymatic catalysis and evolution*
	Physical organic chemistry and catalysis *Room: Margarinfabrikken 1* **Chair: M. Podewitz**	**From picoseconds to attoseconds: Nuclear and electron dynamics** *Room: Margarinfabrikken 2* **Chair: L. Gonzalez**	**Ultracold chemical physics** *Room: Margarinfabrikken 3* **Chair: B. Jeziorski**	
14:00	**Satoshi Maeda** *Systematic Generation and Analysis of Reaction Path Networks by the Artificial Force Induced Reaction Method*	**Fernando Martin** *Attosecond pump-probe spectroscopy of molecular electron dynamics*	**Guido Pupillo** *Cavity-induced collective dissipation for cold chemistry*	
14:30	**Natalie Fey** *CatLab – Putting calculation before experiment in organometallic catalysis*	**Eberhard Gross** *Potential energy surfaces and Berry phases from the exact factorization: A rigorous approach to non-adiabatic dynamics*	**Olivier Dulieu** *Ultracold doubly-polar molecules: on the way to create them via a Laser-Assisted Self-Induced Feshbach Resonance*	
15:00	**Markus Reiher** *Quantum Chemical Exploration of Catalytic Reaction Networks*	**Nina Rohringer** *Stimulated X-Ray Emission Spectroscopy for Chemical Analysis*	**Robert Moszynski** *New physics with ultracold strontium molecules*	
15:30	**Heather J. Kulik** *Transition metal catalyst discovery with high-throughput screening and machine learning*	**Boutheina Kerkeni** *Understanding H2 Formation on hydroxylated nanopyroxene clusters: Ab initio Study of the Reaction Energetics and Kinetics*	**Svetlana Kotochigova** *Nonadiabatic Transitions via Conical Intersections in Ultracold Chemical Reactions*	
	Computational spectroscopy: from X-rays to microwaves *Room: Margarinfabrikken 1* **Chair: B. Durbeej**	**Emergent electronic structure methods** *Room: Margarinfabrikken 2* **Chair: S. Goedecker**	**Path-integral methods** *Room: Margarinfabrikken 3* **Chair: D. Manolopoulos**	
16:30	**Julien Bloino** *A Virtual Spectrometer to Predict and Interpret Vibrational Spectra*	**Steven R. White** *Multisliced Gausslet Bases for Electronic Structure*	**Barak Hirshberg** *Path Integral Molecular Dynamics for Bosons*	
17:00	**Tucker Carrington** *Collocation methods for computing vibrational spectra*	**Garnet Chan** *Progress in quantum embedding in the condensed phase*	**Seogjoo Jang** *Quantum Fokker-Planck equation with positive definiteness condition via path integral influence functional formalism*	
17:30	**Ad van der Avoird** *Spectra of O2 induced by collisions with N2 and O2*	**Philippe Corboz** *Simulation of strongly correlated systems with 2D tensor networks*	**Pierre-Nicholas Roy** *Quantum dynamics of confined molecules*	
18:00	**Fabien Gatti** *The polyspherical approach: recent applications to spectroscopy*	**Örs Legeza** *Attosecond electron dynamics via tensor network state methods in strongly correlated molecular systems*	**Gregory A. Voth** *Coarse-graining of Feynman Path Integrals in Statistical Mechanics*	
19:00	**Poster session 2**			
	Posters 1-14: On the walls outside *Margarinfabrikken 1+2+3*	**Posters 25-42:** In the meeting room *Prostneset*	**Posters 59-74:** In the meeting room *Kjøpmannskontoret*	
	Posters 15-24: On the walls of the meeting room *Skarven*	**Posters 43-58:** In the meeting room *Importkompaniet*	**Posters 75-139:** In the room *Arbeidskontoret 1+2*	

Tuesday, July 16	Plenary lectures *Room: Margarinfabrikken 1+2+3* **Chair: D. Crawford**			
8:30	**Giulia Galli** *Simulating energy conversion processes from first principles*			
9:15	**Zhigang Shuai** *Density matrix renormalization group: time-dependent formalism, light-emitting, carrier transport, and singlet fission*			
	Physical organic chemistry and catalysis *Room: Margarinfabrikken 1* **Chair: O. Eisenstein**	**Large-scale electronic structure models of materials** *Room: Margarinfabrikken 2* **Chair: M. Mayes**	**Ultracold chemical physics** *Room: Margarinfabrikken 3* **Chair: J. Hutson**	**Janos Ladik memorial symposium** *Room: Arbeidskontoret* **Chair: A. Bende**
10:30	**Yousung Jung** *Catalysts Discovery and Understanding with Computational and Data-Driven Approaches*	**Helio A. Duarte** *Unveiling the chemical reactivity of sulfide mineral surfaces in the presence of water and oxygen*	**Paul Julienne** *Calculations of three body recombination and dimer product distributions from ultracold atomic collisions*	**Rodney J. Bartlett** *The devil's triangle in KS-DFT calculations and how to fix it*
11:00	**Carine Michel** *Modeling reactivity at the catalyst/water interface*	**Johannes Neugebauer** *Exact Subsystem Time-Dependent Density-Functional Theory*	**John Bohn** *Ultracold Collisions of Polyatomic CaOH Molecules*	**Alia Tadjer** *Molecular modelling of hybrid-ion batteries*
11:30	**Hai Lin** *Simulations of Ion Solvation and Transfer by Adaptive-Partitioning QM/MM Dynamics*	**Marcus Elstner** *Multi-scale methods for electron and exciton transfer in biological and organic materials*	**Robin Cote** *Optical production of polyatomic complex in ultracold regime*	**Martin Quack** *Fundamental and approximate symmetries, parity violation and tunnelling in chiral and achiral molecules*
12:00	**Michelle Coote** *Catalyzing and Controlling Chemical Reactions with Electric Fields*	**Tsuyoshi Miyazaki** *Linear-scaling DFT simulations of complex nano-structured materials using the CONQUEST code*	**Tijs Karman** *Collisional loss of ultracold molecules*	**Cleanthes Nicolaides** *Attosecond-resolved Quantum Chemistry. Predictions from the early years and comparison with recent experiments*
	Emergent electronic structure methods *Room: Margarinfabrikken 1+2* **Chair: C. Hättig**	**Computational spectroscopy: from X-rays to microwaves** *Room: Margarinfabrikken 3* **Chair: V. Liegeois**	**Computational biophysics** *Room: Arbeidskontoret* **Chair: B. Brandsdal**	
14:00	**Michiel van Setten** *Benchmarking GW for quantum chemistry applications*	**Faris Gelmukhanov** *X-ray Raman scattering of liquids*	**Inaki Tunon** *Quantum Hydride Transfer in Formate Dehydrogenase: Environment Reorganization and Primary and Secondary Hydrogen Motions*	
14:30	**Stefan Goedecker** *Wavelets for electronic structure calculations, an introduction and overview*	**Vincenzo Carravetta** *Aqueous solutions: a look at the surface*	**Maria Joao Ramos** *Understanding enzymatic reactions*	
15:00	**Luigi Genovese** *Potentialities of Wavelet formalisms for large-scale DFT calculations and beyond*	**Barbara Brena** *Calculation of X-Ray Absorption and Photoemission Spectra of Molecules in Complex Environment*	**Qiang Cui** *QM/MM analysis of metalloenzymes: developments and applications*	
15:30	**Luca Frediani** *MRChem: Quantum Chemistry at the basis set limit with Multiwavelets*	**Weijie Hua** *Computational optical and X-ray spectroscopy studies for crystals & 2D materials*	**Fernanda Duarte Gonzalez** *Unraveling the Role of Non–Covalent Interactions in Recognition and Catalysis*	
	Large-scale electronic structure models of materials *Room: Margarinfabrikken 2* **Chair: H. Nakai**	**From picoseconds to attoseconds: Nuclear and electron dynamics** *Room: Margarinfabrikken 3* **Chair: F. Martin**	**Ultracold chemical physics** *Room: Arbeidskontoret* **Chair: P. Julienne**	
16:30	**Woo Youn Kim** *Efficient hybrid density functional calculations in real-space numerical grid methods*	**David Clary** *Quantum Tunnelling in Chemical Reactions*	**Rosario Gonzalez-Ferez** *Rydberg polyatomic molecules: Electronic structure and experimental proposal for their creation*	
17:00	**Beatriz Gonzalez del Rio** *Large-scale Ab Initio Simulations with Orbital-free Density Functional Theory*	**Francoise Remacle** *Spatial and temporal localization of the vibronic and photoelectron wave packets in LiH photoexcited by intense few cycle IR pulses*	**Timur Tscherbul** *Magnetic tuning of ultracold chemical reactions: Theoretical insights*	
17:30	**Damiano Marian** *Multi-scale approach: a versatile platform for investigating novel two-dimensional-material based device concepts*	**Olga Smirnova** *Synthetic chiral light for extremely efficient laser-controlled chiral discrimination*	**Christiane Koch** *Quantum effects in cold and controlled molecular dynamics*	
18:00	**David Tomanek** *Magic with Semiconducting 2D Nanolayers*	**Morgane Vacher** *Insights into chemiluminescence from molecular dynamics simulations and machine learning analysis*	**Goulven Quemener** *Shielding ultracold molecules against losses in collision*	
20:30	**Conference dinner** *Room: Margarinfabrikken 1+2+3*			

Wednesday, July 17	Computational spectroscopy: from X-rays to microwaves *Room: Margarinfabrikken 1+2* **Chair: A. Csaszar**	Computational biophysics *Room: Margarinfabrikken 3* **Chair: F. Duarte**	Janos Ladik memorial symposium *Room: Arbeidskontoret* **Chair: K. Ruud**
8:30	**Csaba Fabri** *From High-Resolution Spectroscopy to Light-Dressed Molecules*	**Rafael Bernardi** *NAMD as a tool for in silico force spectroscopy*	**Mark Hoffman** *Multireference Configuration Interation Beyond Singles and Doubles*
9:00	**Cristina Puzzarini** *Rotational Spectroscopy Meets Quantum Chemistry for Elucidating Astrochemical Challenges*	**Michele Vendruscolo** *Systematic development of small molecules to inhibit amyloid beta aggregation in Alzheimer's disease*	**Hazel Cox** *The Limits of Stability in Three-Body Coulomb Systems*
9:30	**Sandra Luber** *Recent developments in dynamic spectroscopic methods for the gas and condensed phase*	**Ramon Crehuet** *Stabilization of α-helices by side-chain to main hydrogen bonds. Can current force fields describe the hydrophobic shielding?*	**Samantha Jenkins** *Beyond Scalar Measures: Directional Chemical Perspective with Next Generation QTAIM*
	Plenary lectures *Room: Margarinfabrikken 1+2+3* **Chair: E. Brändas**		
10:30	**Monica Olvera de la Cruz** *Properties of Molecular Electrolytes*		
11:15	**Kersti Hermansson** *OH, ceriously, ... Molecules + materials = difficult!*		