Grand Challenges for Theoretical Chemistry (GCTC)

A conference on the occasion of Prof. Dr. Scient. Kurt V. Mikkelsen's 60th birthday

Time	Monday 19th Damgaardsalen	Tuesday 20th Damgaardsalen	Wednesday 21st Øresundssalen
9:00 - 9:30	Arrival	**Chairman: Ove Christiansen** **Sylvio Canuto** Free Energy Gradient method with Average Solvent Electrostatic Configuration for Studying Electronic Properties of Molecules in Solution and in Complex Environment	**Chairman: Patrick Norman** **Kaline Coutinho** Conformational Bias Monte Carlo Used to Study the Solvatochromism of Mesityl Oxide
9:30 - 10:00		**Steen Brøndsted Nielsen** Protein biochromophores: What affects their absorption and luminescence?	**Klaus Braagaard Møller** Solvent and solvent-influenced dynamics in theoretical chemistry
10:00 - 10:30		**Jógvan Magnus Haugaard Olsen** Development of Multiscale Methods for Computational Biomolecular Spectroscopy	**Kestutis Aidas** Molecular aggregation in glacial acetic acid: insight from molecular dynamics/quantum mechanics modelling of structural and H-1 NMR properties
10:30 - 11:00		Break	Break
11:00 - 11:30		**Chairman: Peter Ogilby** **Merete Bilde** Atmospheric Aerosols – a multifaceted challenge	**Chairman: Kenneth Ruud** **Lasse Jensen** Spectroscopy in Inhomogeneous Fields
11:30 - 12:00		**Matthew S. Johnson** Innovation and Atmospheric Science	**Frank Jensen** Describing force field polarization by a bond capacity model
12:00 - 12:30	Lunch	**Jonas Elm** Modelling the Formation and Properties of Atmospheric Molecular Clusters	**Jens Ulstrup** The Au-Sulfur Bond in Electrochemistry and *In Situ* Scanning Tunnelling Microscopy
12:30 - 13:00		Lunch	Lunch
13:00 - 13:30	**13:15 Welcome**		
13:30 - 14:00	**Chairman: Sylvio Canuto** **Marshall Newton** Recent challenges and some thoughts regarding charge transfer mechanisms, both homogeneous and interfacial	**Chairman: Jeppe Olsen** **Poul Jørgensen** Cluster perturbation theory. A new wave function model in electronic structure theory	**Chairman: Hans Ågren** **Allan Gross** New Directions in Development of Complex Stiff Chemical Schemes (CSCS)
14:00 - 14:30	**Henrik G. Kjærgaard** Accurate calculation of vibrational transition in a reduced dimensionality model	**Henrik Koch** Recent developments in coupled cluster theory and perspectives for the future	**Mads Koerstz** Chemical Space Exploration
14:30 - 15:00	**Ove Christiansen** New time-dependent wave functions methods: Second Quantization based Time-dependent Hartree and Multi-Configurational extensions and Time-dependent Vibrational Coupled Cluster	**Thomas B. Pedersen** Can coupled-cluster theory describe ultrashort, high-intensity laser-driven electron dynamics?	**Zilvinas Rinkevicius** Quantum chemistry on modern HPC systems: challenges and opportunities
15:00 - 15:30	**Kasper Moth-Poulsen** Molecular solar thermal systems	**Sonia Coriani** Coupled Cluster methods for X-ray spectroscopies	**Theo Kurten** Self-reactions of peroxy radicals: overturning the 60-year old Russell mechanism
15:30 - 16:00	Break	Break	Break
16:00 - 16:30	**Chairman: Jan Linderberg** **Trygve Helgaker** Robust optimization of the density in orbital-free density-functional theory	**Chairman: Allan Gross** **Patrick Norman** An unfinished affair with Mikkelsen	Departure
16:30 - 17:00	**Hans Jørgen Aagaard Jensen** Status and perspectives for the multiconfigurational short-range density functional theory method	**Jeppe Olsen** The development and use of wave functions with several sets of optimised orbitals	
17:00 - 17:30	**Kenneth Ruud** Relativistic DFT with periodic boundary conditions	**Peter R. Ogilby** The Oxygen-Organic Molecule Photosystem: Tunneling through Activation Barriers	
17:30 - 18:00	**Hans Ågren** Three things Kurt needs to do before it is too late...	**Mogens Brøndsted Nielsen** Tuning Molecular Properties of the Dihydroazulene/Vinylheptafulvene Photo/Thermoswitch	
19:00 - 20:30 20:30	Dinner **Poster session**	**Conference Dinner**	