MEAL 2018 PROGRAM

Thursday, December 13, 2018

12:30 – 13:25		Arrival & registration in the foyer
13:25 – 13:30		Welcome and introductory remarks by the organizers
13:30 – 13:35	Session I Auditorium I	**Session I chair: Jack Simons**
13:35 – 14:00		**Josef Michl**, University of Colorado, USA and Academy of Sciences of the Czech Republic *Singlet Fission*
14:00 – 14:25		**Sonia Coriani**, Technical University of Denmark *Theoretical Beamlines for Modern Spectroscopic Experiments*
14:25 – 14:50		**Hans Jørgen Aagaard Jensen**, University of Southern Denmark *Status and Perspectives for MC-srDFT*
14:50 – 15:15		**Lars Bojer Madsen**, Aarhus University, Denmark *Wave function based approaches to the time-dependent many-electron problem*
		Coffee break
15:45 – 15:50	Session II Auditorium I	**Session II chair: Esper Dalgaard**
15:50 – 16:15		**Daniel Crawford**, Virginia Tech, USA *Streamlining coupled-cluster response theory*
16:15 – 16:40		**Filip Pawlowski**, Auburn University, USA *Cluster perturbation theory*
16:40 – 17:05		**Pablo Baudin**, École Polytechnique Fédérale de Lausanne, Switzerland *CCSD excitation energies for large systems: the CPS(D-3) model*
17:05 – 17:30		**Lars Henrik Andersen**, Aarhus University, Denmark *The use of ion-storage rings for action spectroscopy of biochromophores.*

Friday, December 14, 2018

9:00 – 9:05	Session III Auditorium I	**Session III chair: Jan Linderberg**
9:05 – 9:30		**Trygve Helgaker**, University of Oslo, Norway *Closed-shell molecular paramagnetism*
9:30 – 9:55		**Antonio Rizzo**, Consiglio Nazionale delle Ricerche, Pisa, Italy *Electronic nonlinear spectroscopic properties: Theory meeting experiment An account of more than 20 years of science, coffee and cake in Aarhus*
9:55 – 10:20		**Rika Kobayashi**, Australian National University, Australia *High Performance Computational Chemistry*
10:20 – 10:45		**Branislav Jansik**, IT4Innovations National Supercomputing Center, Czech Republic *On the path to exascale computing: outlooks and challenges*
		Coffee break

11:00 – 11:05	Session IV Auditorium I	**Session IV chair: Poul Jørgensen**
11:05 – 11:30		**Angela Wilson**, Michigan State University, USA *Energetic and Spectroscopic Properties: Methodologies for the Transition Metals and Beyond*
11:30 – 11:55		**Kurt Valentin Mikkelsen**, University of Copenhagen, Denmark *Exploitation of Solar Energy*
11:55 – 12:20		**Dage Sundholm**, University of Helsinki, Finland *Efficient Algorithms for Numerical Electronic Structure Calculations on Molecules*
	Lunch	
13:30 – 13:35	Session V Auditorium I	**Session V chair: Jeppe Olsen**
13:35 – 14:00		**Erik Hedegaard**, Lund University, Sweden *Embedding for the entire periodic table*
14:00 – 14:25		**Ida-Marie Høyvik**, Norwegian University of Science and Technology, Norway *The multilevel Hartree-Fock model*
14:25 – 14:50		**Janus Juul Eriksen**, Johannes Gutenberg-Universität Mainz, Germany *Many-Body Expanded Full Configuration Interaction*
14:50 – 15:15		**Nanna List**, Stanford University, USA *Nonadiabatic dynamics*
	Coffee & Cake	
15:45 – 15:50	Session VI Auditorium I	**Session VI chair: Ove Christiansen**
15:50 – 16:15		**Christof Hättig**, Ruhr-University Bochum, Germany *Excited state potential energy surfaces in polarizable environments with correlated wavefunction methods*
16:15 – 16:40		**Gunnar Schmitz**, Aarhus University, Denmark *Enhancing Quantum Chemical Algorithms: Compress, rethink, be lazy and combine*
16:40 – 17:05		**Stephan P.A. Sauer**, University of Copenhagen, Denmark *RPA(D) and HRPA(D): two new models for the calculation of linear response properties*
17:05 –	Poster session & refreshments	

Saturday, December 15, 2018

9:00 – 9:05	Session VII Auditorium I	**Session VII chair: Kurt V. Mikkelsen**
9:05 – 9:30		**Markus Reiher**, Swiss Federal Institute of Technology in Zurich, Switzerland *Vibrational Density Matrix Renormalization Group*
9:30 – 9:55		**Carolin König**, Kiel University, Germany *Pushing the size limitations of anharmonic vibrational spectra calculations*
9:55 – 10:20		**Berta Fernández Rodríguez**, University of Santiago de Compostela, Spain *Improving the accuracy of intermolecular potential energy surfaces and rovibrational spectra of weak-bonded complexes.*

10:20 – 10:45		**Patrick Norman**, KTH Royal Institute of Technology, Sweden *VeloxChem: a highly modular Python-driven software initiative for spectroscopic properties of complex molecular systems*
	Coffee break	
11:00 – 11:05	Session VIII Auditorium I	**Session VIII chair: Trygve Helgaker**
11:05 – 11:30		**Kenneth Ruud**, UiT The Arctic University of Norway *To be announced*
11:30 – 11:55		**Roland Lindh**, Uppsala University, Sweden *Ab Initio calculation on muonic atoms and molecules*
11:55 – 12:20		**Sarai Dery Folkestad**, Norwegian University of Science and Technology, Norway *Efficient Cholesky decomposition algorithms for multilevel methods*
	Lunch	
13:30 – 13:35	Session IX Auditorium I	**Session IX chair: Hans Jørgen Aagaard Jensen**
13:35 – 14:00		**Trond Saue**, Université Toulouse III-Paul Sabatier, France *X2C as an effective Hamiltonian*
14:00 – 14:25		**Willem Klopper**, Karlsruhe Institute of Technology, Germany *Bethe-Salpeter correlation energies of atoms and molecules*
14:25 – 14:50		**Mikael Johansson**, University of Helsinki, Finland *Effect of reference function on approximate coupled cluster*
	Coffee & Cake	
15:20 – 15:25	Session X Auditorium I	**Session X chair: Danny Yeager**
15:25 – 15:50		**Thomas Bondo Pedersen**, University of Oslo, Norway *Electron dynamics with coupled-cluster theory*
15:50 – 16:15		**Peter Knowles**, Cardiff University, Wales, UK *Orbital optimisation and Fock operators in coupled-cluster theory*
16:15 – 16:40		**Christian Ochsenfeld**, Ludwig-Maximilians-Universität München, Germany *Linear- and low-scaling calculation of direct and beyond RPA correlation energies*
16:40 – 16:45	Closing remarks by the organizers	
18:00	Aperitif in the Canteen	
18:30	Conference Dinner in the Canteen	