

TRAINS

time table



Monday, nov. 27

12:30-14:00	Lunch
14:00-14:05	Opening
14:05-14:15	Honorary speech by Knut Fægri

Session 1 (Chair: Pedersen)

14:15-14:45	The Molecular Physics lecture: Poul Jørgensen <i>Cluster perturbation theory</i>
14:45-15:15	Trond Saue <i>Beyond the Dailey-Townes model: chemical information from the electric field gradient</i>
15:15-15:45	Hans Jørgen Aa. Jensen <i>Multiconfiguration Short-Range Density Functional Theory: Status and Perspectives</i>

15:45-16:05	Coffee break
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Session 2 (Chair: Frediani)

16:05-16:35	Hans-Joachim Werner <i>The p-block challenge: explicitly correlated local coupled cluster studies of inorganic heterocycles</i>
16:35-17:05	Ove Christiansen <i>Direct Quantum Molecular Dynamics</i>
17:05-17:35	Elke Fasshauer <i>How nuclear degrees of freedom influence time-resolved spectroscopy of electronic decay processes</i>

Break

18:45	Dinner
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Tuesday, nov. 28

Session 3 (Chair: Stopkowicz)

9:00-9:30	Wim Klopper <i>Explicitly-correlated second-order correction to the GW approximation</i>
9:30-10:00	Hans-Peter Lühti <i>A Look Back and a Look Forward: The Bright Side of Failure</i>
10:00-10:30	Andre Laestadius <i>Can we make the exchange energy virial?</i>

10:30 - 11:00	Coffee break (with pastry)
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Session 4 (Chair: Christiansen)

11:00-11:30	Jürgen Gauss <i>Recent Advances in the Use of Cholesky Decomposition within Electron-Correlated Calculations of Energy and Properties</i>
11:30-12:00	Henrik Koch <i>Recent developments of ab initio QED methods</i>
12:00-12:30	Sarai Folkestad <i>Entanglement coupled cluster theory for open-shell systems</i>

12:30 - 14:00	Lunch
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Session 5 (Chair: Saue)

14:00-14:30	Hans Ågren <i>Coherent and incoherent upconversion</i>
14:30-15:00	Ida-Marie Høyvik <i>Molecules as electronically open quantum systems</i>
15:00-15:30	David Tew <i>A spin-coupled orbital theory for molecular bonding</i>

15:30 - 16:00	Coffee break
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Session 6 (Chair: Eisenstein)

16:00-16:30	David J. Tozer <i>Two studies in DFT</i>
16:30-17:00	Vladimir Rybkin <i>Understanding radicals via orbital parity</i>
17:00-17:30	Peter Schmelcher <i>Ultralong-Range Molecules: Exotic molecules on exaggerated scales</i>

Break

18:30-19:30	Poster session
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19:45	Dinner
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Wednesday, nov. 29

Session 7 (Chair: Tellgren)

9:00-9:30	Andrew Wibowo-Teale <i>Keeping it simple: Can xTB approaches describe molecules in strong magnetic fields?</i>
9:30-10:00	Stella Stopkowicz <i>A (strongly magnetic) train-ride in highly-accurate electronic structure</i>
10:00-10:30	Anand Thirumalai <i>Strange stars and even stranger chemistry</i>

10:30-11:00 Coffee break (with pastry)

Session 8 (Chair: Taylor)

11:00-11:30	Antonio Rizzo <i>Multiphoton Optical Rotation That was missing, wasn't it?</i>
11:30-12:00	Kurt V. Mikkelsen <i>The Times They Are A-Changin'</i>
12:00-12:30	Einar Uggerud <i>The Factors that Determine Reactivity in Nucleophilic Substitution</i>

12:30-14:00 Lunch

Session 9 (Chair: Wibowo-Teale)

14:00-14:30	Sonia Coriani <i>TRAINS' legacy on my own journey: from spectroscopy to quantum computing</i>
14:30-15:00	Daniel Crawford <i>Reduced-Scaling Coupled Cluster Response Theory in the Frequency and Time Domains</i>
15:00-15:30	Stephan Sauer <i>Aspects of the calculation of NMR spin-spin coupling constants</i>

15:30-16:00 Coffee break

Session 10 (Chair: Rizzo)

16:00-16:30	Kenneth Ruud <i>TRAINS in multiple dimension</i>
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Break

16:40-17:30 NKS general assembly (for members of the Norwegian Chemical Society)

Break

18:30 Banquet (apertiff at 18:30, dinner from 19:00)

Thursday, nov. 30

Session 11 (Chair: Tellgren)

9:00-9:30	Peter R. Taylor <i>Crossing paths</i>
9:30-10:00	Mark R. Hoffman <i>Optimization Using Riemannian Manifolds</i>
10:00-10:30	Luca Frediani <i>A journey on the Multiwavelet train in a Quantum Chemistry landscape</i>

10:30-11:00 Coffee break (with pastry)

Session 12 (Chair: Cascella)

11:00-11:30	Odile Eisenstein <i>Going North: A french chemist in TheoryLands</i>
11:30-12:00	Andreas Savin <i>Density functional theory without density functionals</i>
12:00-12:30	Simen Kvaal <i>Development of multireference coupled-cluster methods from singlestate and multistate bivariational principles</i>

12:30-12:40 Closing
12:40-14:00 Lunch