

# PROGRAM “Open shells, open questions”

Monday August 24

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*Afternoon session. Chairman: Trond Saue*

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- 14:50** *Words of welcome and practical information*
- 15:00** Vladimir Malkin: **Calculations of the EPR g-tensor in the framework of 2- and 4-component DFT approaches**
- 15:30** H el ene Bolvin: **EPR and pNMR parameters for actinide compounds**
- 16:00** Stephan P. A. Sauer: **Exploring the limits of Coupled Cluster calculations of NMR coupling constants**
- 16:30** *Coffee break*
- 17:00** Christel Marian: **Redesigned DFT/MRCI**
- 17:30** Julien Toulouse: **Combining many-body methods and density-functional theory**
- 18:00** Emmanuel Fromager: **Site-occupation embedding theory**
- 20:00** *Dinner*

Tuesday August 25

**07:00 – 09:00** *Breakfast buffet*

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*Morning session. Chairman: Peter Taylor*

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- 09:00** Simen Kvaal: **The Bivariational Principle and Coupled-Cluster Theory**
- 09:30** Ephraim Eliav: **Relativistic mixed-sector coupled cluster method: recent developments and applications**
- 10:00** Flemming J orgensen: **Geometry of Van Vleck’s transformation to an effective Hamiltonian**
- 10:30** *Coffee break*
- 11:00** Lucas Visscher: **Electron correlation and spin-orbit coupling, the challenge of f-elements.**
- 11:30** Stefan Knecht: **The electron correlation problem in the lower part of the periodic table**
- 12:00 - 14:00** *Lunch buffet*

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*Afternoon session. Chairman: Nanna Holmgaard List*

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- 14:00** Michal Repisky: **Molecular Properties from Relativistic Real-Time Time-Dependent Density Functional Theory Calculations**

- 14:30** Sonia Coriani: **News from the CC world: xray absorption spectroscopy, ionization and (maybe) more**
- 15:00** Marcus Lundberg: **Multiconfigurational descriptions of transition metal X-ray spectra**
- 15:30** Patrick Norman: **Beyond the electric-dipole approximation: A formulation and implementation of molecular response theory for the description of absorption of electromagnetic field radiation**
- 16:00** *Coffee break*
- 16:30** Toru Shiozaki: **Fully relativistic quantum chemistry for large Open Shells**
- 17:00** Markus Reiher: **The Choice of the Active Space in DMRG Calculations**
- 17:30** Jeppe Olsen: **Novel methods for Configuration Interaction and Orbital Optimization for Non-orthogonal expansions with Applications to the Chromium Dimer and Trimer**
- 18:00** Hans Jørgen Aagaard Jensen: **Open Shells, Open Questions**
- 20:00** *Dinner*

**Wednesday August 26**

**07:00 – 09:00** *Breakfast buffet*

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*Morning session. Chairman: Stanislav Komarovskiy*

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- 09:00** Timo Fleig: **In Search of Physics Beyond the Standard Model. LUCI\* in the Sky with Diamonds**
- 09:30** Poul Jørgensen: **Coupled Cluster Perturbation Theory**
- 10:00** Debashis Mukherjee: **Unitary Group Adapted MRCC and MRPT Theories: SU vs SS Approaches**
- 10:30** *Coffee break*
- 11:00** Hans Ågren: **A gammeldansk in good spirits**
- 11:30** Kenneth Ruud: **New advances and open questions in modeling multidimensional spectroscopy**
- 12:00 - 14:00** *Lunch buffet*

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*Afternoon session. Chairman: Jacob Kongsted*

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- 14:00** Trygve Helgaker: **Density-functional theory in magnetic fields**
- 14:30** Jan Linderberg: **Exchange in a Dirac-Fermi-Thomas world**
- 15:00** Andreas Savin: **Do we know what spin-density means in density functional approximations?**
- 15:30** Martin Kaupp: **Local hybrid functionals: towards a useful practical tool**

**16:00** *Coffee break*

**16:30** Erik Donovan Hedegård: **Exploring Large Systems with Multiconfigurational Wave Functions**

**17:00** Kurt Mikkelsen: **Sirius Applications and Capture of Solar Energy**

**17:30** Frank Jensen: **Force Field Electrostatics**

**20:00** *Conference Dinner*

