

Program

Tuesday, May 4

15.00-
19.00

Registration

15.30

Coffee

19.30-
20.30

Dinner

20.45-
21.00

Late registration

Wednesday, May 5

| | | |
|-----------------|------------------|---|
| 08.00- 08.45 | | <i>Breakfast</i> |
| 08.45 | H. J. Aa. Jensen | <i>Welcoming address</i> |
| 09.00 | R. J. Bartlett | Some Considerations of Response Functions, Excited States, and Triple Excitations |
| 09.30 | T. D. Crawford | Local correlation in coupled cluster response theory |
| 10.00 | C. Hättig | Optimization of excited state structures with correlated second-order methods: CC2 and ADC(2) |
| 10.30 | | <i>Coffee break</i> |
| 10.50 | H. Koch | Reduced scaling in electronic structure calculations |
| 11.20 | F. Harris | New Methods for Old Coulomb Few-Body Problems |
| 12.00- 13.00 | | <i>Lunch</i> |
| 13.30 | S. van Gisbergen | Analytic evaluation of molecular properties in DFT and TDDFT: Examples from ADF |
| 14.00 | O. Vahtras | Density functional response theory with applications to open-shell systems |
| 14.30 | N. Handy | A new hybrid exchange-correlation functional using the Coulomb-Attenuating Method (CAM-B3LYP) |
| 15.00 | | <i>Coffee break</i> |
| 15.30 | N. Y. Öhrn | Time-Dependent Molecular Reaction Dynamics |
| 16.00 | M. A. Ratner | Molecular junction transport: Structure, tunneling, conductance and a bit beyond |
| 16.30 | J. Simons | The Response of DNA to Low-Energy Electrons |
| 17.00 | H. Ågren | Dynamics of Pulse Propagation in Nonlinear Media |
| 18.00- 19.00 | | <i>Dinner</i> |

Thursday, May 6

| | | |
|-----------------|------------------|---|
| 08.00- 08.50 | | <i>Breakfast</i> |
| 08.50 | H. J. Aa. Jensen | <i>Practical remarks</i> |
| 09.00 | J. Schirmer | Electronic excitation in molecules: From propagator theory to intermediate state representations |
| 09.30 | J. V. Ortiz | Insights into Chemical Bonding from Electron Propagator Theory |
| 10.00 | N. Y. Öhrn | <i>Jan Linderberg, Scientist, Teacher, Friend</i> |
| 10.30 | | <i>Coffee break</i> |
| 10.50 | J. E. Del Bene | Two-bond spin-spin coupling constants (${}^2hJ(X-Y)$] across X-H-Y hydrogen bonds: Some fundamental questions |
| 11.20 | S. P. A. Sauer | Correlated ab initio calculations of NMR spin-spin coupling constants |
| 12.00- 13.00 | | <i>Lunch</i> |
| 15.00 | | <i>Coffee</i> |
| 15.30 | T. Saue | Spin-interactions and the non-relativistic limit of electrodynamics |
| 16.00 | B. Roos | Heavy Element Quantum chemistry - the Multiconfigurational Approach |
| 16.30 | M. Urban | Some trends in relativistic and electron correlation effects in electric properties of small molecules |
| 17.00 | L. Visscher | Methods to include relativity and electron correlation in the calculation of molecular properties |
| 18.00- 19.00 | | <i>Dinner</i> |
| 20.00- 22.00 | | Poster session |

Friday, May 7[†]

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|-------------|------------------|---|
| 08.00-08.50 | | <i>Breakfast</i> |
| 08.50 | H. J. Aa. Jensen | <i>Practical remarks</i> |
| 09.00 | M. Jaszuński | Helium dimer interaction energies |
| 09.30 | D. L. Yeager | A Quadratically Convergent Multiconfigurational Self Consistent Field Method for Complex Scaled Hamiltonians |
| 10.00 | J. Oddershede | <i>Poul Jørgensen and his science</i> |
| 10.30 | | <i>Coffee break</i> |
| 10.50 | K. V. Mikkelsen | JP operators and solvent models |
| 11.20 | K. Ruud | Solvents effects on magnetic properties using the polarizable continuum model |
| 12.00-13.00 | | <i>Lunch</i> |
| 14.00 | D. Bishop | Aspects of nonlinear optical calculations: From the Hydrogen atom to infinite chain polymers |
| 14.30 | Y. Luo | Multi-photon Absorption of Molecules |
| 15.00 | A. Rizzo | Benchmarking on electric and magnetic high order molecular properties |
| 15.30 | D. Sundholm | Magnetic and optical properties of molecular clusters |
| 16.00 | | <i>Coffee break</i> |
| 16.30 | T. Helgaker | The application of response theory to large molecular systems |
| 17.00 | J. Gauss | Rovibrational Spectroscopy and Quantum Chemistry |
| 17.30 | K. J. Jalkanen | A study of the energetics, structures and vibrational spectra of [Leu]enkephalin based on SCC-DFTB, B3LYP, AM1, PM3, and Charmm force field methodologies |
| 18.00 | J. Olsen | <i>Concluding remarks</i> |
| 19.00 | | <i>Conference dinner</i> |

[†]This Friday is a Holiday in Denmark, "Store Bededag", and most shops are closed.

Saturday, May 8

08.00-
09.00

Breakfast

Departure
