# Theoretical Chemistry Seminar WS 2006/07

| WS 2006/07 | | |
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| **Date**<br>**Time** | **Title**<br>**Speaker** | **Place** |
| 18.10.2006<br>9.00 | Calculation of NMR Chemical Shifts Using Frozen-Density Embedding<br>Christoph Jacob | HCI-J243<br>(ETH) |
| 08.11.2006<br>9:00 | Density functional investigation of carbonic anhydrase model systems<br>Stephan Schenk | HCI-J243<br>(ETH) |
| 15.11.2006<br>9:00 | Cholesky decomposition of the two-electron integrals: A reliable tool for reduced scaling methods?<br>Roland Lindh | HCI-J243<br>(ETH) |
| 22.11.2006<br>9:00 | Pyrimidine Dimer Photorepair by DNA Photolyase: An Update IV<br>Fanny Masson | 34-K-01<br>(Uni) |
| 29.11.2006<br>9:00 | Numerical integration of a nonlocal operator: Some results<br>Thomas Kastl | 34-K-01<br>(Uni) |
| 06.12.2006<br>9:00 | Continous-Time Simulation of Dissipative Quantumsystems<br>Manuel Guidon | 34-K-01<br>(Uni) |
| 13.12.2006<br>9:00 | Relativistic calculations of g-tensors and hyperfine coupling constants<br>Irina Malkin Ondik | HCI-J243<br>(ETH) |
| 20.12.2006<br>9:00 | Chemoinformatics Approaches for Solving Practical Problems in Chemistry: Attempts to Predict Reactions and Structures<br>Hirako Satoh | HCI-J243<br>(ETH) |
| 10.01.2007<br>9:00 | A Core-Extensive Solution to the Multi-Reference Coupled Cluster Problem<br>Michael Hanrath | HCI-J243<br>(ETH) |
| 17.01.2007<br>9:00 | DFT studies of adsorption of aromatics on metal clusters<br>Gianluca Santarosa | 34-K-01<br>(Uni) |
| 24.01.2007<br>9:00 | On the nature of ligand-induced charge concentrations in transition-metal complexes<br>Georg Eickerling | HCI-J243<br>(ETH) |
| 31.01.2007<br>9:00 | *to be announced*<br>Florian Schiffmann | 34-K-01<br>(Uni) |
| 07.02.2007<br>9:00 | Going from A to B without a map: exploring free energy surfaces<br>Teodoro Laino | 34-K-01<br>(Uni) |
| 14.02.2007<br>9:00 | Classical and Ab Initio Molecular Dynamics Simulations of the Standard Amino Acids in Aqeous Solution<br>Samuele Giani | 34-K-01<br>(Uni) |
| 21.02.2007<br>9:00 | *to be announced*<br>Joost VandeVondele | 34-K-01<br>(Uni) |