Theoretical Chemistry Seminar SS 2006

SS 2006		
Date **Time**	**Title** **Speaker**	**Place**
08.03.06 9:00	Operators in GAPW Jürg Hutter	34-K-01 (Uni)
15.03.06 9:00	System/environment embedding within density functional theory Johannes Neugebauer	HCI-D6 (ETH)
22.03.06 9:00	Approximate MP2 Methods for Intermolecular Interactions? Hans Peter Lüthi	34-K-01 (Uni)
29.03.06 9:00	Lithium Hydroxide Phase Transition under High Pressure Marcella Iannuzzi	34-K-01 (Uni)
05.04.06 9:00	Calculation of first-order properties within the arbitrary-order DKH framework Markus Reiher	HCI-D6 (ETH)
12.04.06 9:00	GEEP: not just QM/MM simulations Teodoro Laino	34-K-01 (Uni)
19.04.06 9:00	A new program for density matrix renormalization group calculations Gerrit Moritz	HCI-D6 (ETH)
26.04.06 9:00	Statistical Analysis of Quantum Chemical Data Using Generalized XML/CML Archives; Part II - The Statistics Andreas Elsner	34-K-01 (Uni)
03.05.06 9:00	First principles Monte Carlo simulations with CP2K Matt McGrath	34-K-01 (Uni)
10.05.06 9:00	On the calculation of Vibrational Raman Optical Activity spectra Carmen Herrmann	HCI-D6 (ETH)
17.05.06 9:00	Light-driven molecular switches: modeling conical intersections from quantum to semiclassical Daniele Passerone	34-K-01 (Uni)
24.05.06 9:00	Pyrimidine Dimer Photorepair by DNA Photolyase: An Update III Fanny Masson	HCI-D6 (ETH)
31.05.06 9:00	On the dynamics of amino acids in their natural environment Samuele Giani	34-K-01 (Uni)
07.06.06 9:00	Molecular dynamics simulations of CaCl2 aqueous solutions Teodora Todorova	HCI-D6 (ETH)
14.06.06 9:00	Tree-methods for long-range potentials Thomas Kastl	34-K-01 (Uni)
21.06.06 9:00	Instability in Jellium: Quagmire in Dirac Exchange Sankha Ghosh	HCI-D6 (ETH)
28.06.06 9:00	Thermal isomerisation of indigo Roger Nadler	34-K-01 (Uni)
05.07.06 9:00	Two components Hartree-Fock: An introduction to relativistic quantum mechanics Florian Schiffmann	HCI-D6 (ETH)