

## Seminar Special Topics in Theoretical Chemistry HS2008

Time: Wednesdays 03:00 pm

Room: HCI J 243

Date	Name	Title
08.10.	Christoph Jacob	PyADF - A scripting framework for quantum chemistry
15.10.	Johannes Neugebauer	Structured Programming with Fortran90
22.10.	Johannes Neugebauer	Structured Programming with Fortran90
29.10.	Lian Yu	Structures of Aryl Calcium Compounds in Ether Solvent
05.11.	Koni Marti	Programming on Cache-Based SMP
12.11.	Karin Kiewisch	Selective Calculation of High-Intensity Vibrations in Molecular Resonance Raman Spectra
19.11.	Martin Stiebritz	Development and Validation of a Protein Design Software
26.11.	Remigius Mastalerz	Spin-Orbit Coupling in Atoms and Linear Molecules
07.01.	Maren Podewitz	Local Spin and Bond Order Terms
14.01.	Villő Pálfi	Self-assembling systems: Collagen and its escape from plaque-formation
21.01.	Samuel Fux	Accurate and Exact Kinetic-Energy Potentials in Orbital-free Density Functional Theory and Frozen Density Embedding
28.01	Christoph Jacob	Localized Vibrations
04.02	Sandra Luber	Towards the theory of vibrational Raman optical activity