

# Special Topics in Theoretical Chemistry

Fall Semester 2011

Time: 13:15

Room: HCI J243

Name	Date	Topic
Benjamin Simmen	27.09.2011	How many Chiral Centers can Raman Optical Activity Spectroscopy Distinguish in a Molecule?
Vasile Catrinel Gradinaru, <i>D-MATH</i>	04.10.2011	Numerical Quantum Dynamics with Semiclassical Wavepackets
Maike Bergeler	18.10.2011	Free energy calculations using DF-TMD: A study of H <sub>2</sub> O <sub>2</sub> and iron complexes in aqueous solution
Moritz Haag	01.11.2011	State of Haptic QC
Paul Johnson, <i>McMaster University</i>	08.11.2011	A Kohn-Sham-Like Model for the 1-Body Reduced Density Matrix
Arndt Finkelmann	15.11.2011	Kinetic Aspects of Reactions at Hydrogenases
Sam Fux	22.11.2011	<del>Au-Mössbauer Spectroscopy</del> - Cancelled
Katharina Boguslawski	29.11.2011	Update on DMRG and Spin Densities
Edit Mátyus	06.12.2011	Progress of Non-BO Theory
Marta Bruska	13.12.2011	Description of Fe <sub>4</sub> S <sub>4</sub> Cubanes
Martin Stiebritz	20.12.2011	The TS Flexibility Model