

## Seminar Special Topics in Theoretical Chemistry HS2010

Time: Wednesdays 02:00 p.m.

Room: HCI J 243

Date	Name	Topic	Exceptions
06.10	Thomas	Can Raman Optical Activity Discriminate Between Different Types of Protein beta-Turns?	
13.10.	Katharina	The DMRG Algorithm in Quantum Chemistry	
20.10.	Sam	Mössbauer Spectroscopy: Theory and Application	
27.10.	Marta	Quantum Chemical Study of the Mechanism of O <sub>2</sub> -induced Inhibition of [FeFe]-Hydrogenase	
03.11.			no group seminar
10.11.	Edit	Quantum chemical computations without clamping the nuclei	
17.11.	Villö	Evaluation of DFT functionals for NMR shielding computations	
24.11.	Steven	The Search for New Ligands in the Catalytic Reduction of Dinitrogen	
01.12.	Noah	Implementation and Evaluation of the Cartesian Transfer Method for Calculating IR, Raman and VROA spectra. The Prag Model	
14.12.	Florian	Trends in VROA-Spectra for Solvating (S)-2-(dimethylamino)-N-methyl-propanamide	
21.12.	no seminar		