

**Special Topics in Theoretical Chemistry**

Reiher Group Seminar • HS 2015

Tuesday, 2:30 p.m., HCI G 232/234

Name	Date	Title
Markus Reiher	Sept. 22	How to Write a Paper
Sebastian Keller	Sept. 29	The Extended Toolset of Maquis DMRG
Arseny Kovyrshin	Oct. 6	Tensor Network Parametrization
Yingjin Ma	Oct. 13	Applying a DMRG-SCF Method to Bioluminescence
Bruno Senjean <sup>a)</sup>		On the Way to an Exact Multiconfigurational DFT in the Orbital Space: Site Occupation Embedding Theory
Jonny Proppe	Oct. 20	Towards a Reliable Computational Protocol for Theoretical Mössbauer Spectroscopy
Adrian Mühlbach		Fast Extrapolation of Density Matrices to Accelerate SCF Calculations [ <i>Master Thesis</i> ]
Andrea Muolo	Oct. 27	Molecular Structure Calculations: Non-Relativistic pre-Born–Oppenheimer Theory
Gregor Simm	Nov. 3	Bayesian Error Estimation for Long-Range Corrected DFT
Tamara Husch	Nov. 10	Semi-Empirical Methods for Transition-Metal Systems
Florian Krausbeck	Nov. 17	Conditional Design of Molecular Scaffolds: An Attempt to Master the Combinatorial Explosion
Stefan Knecht	Nov. 24	Internally Contracted Multireference PT <sub>2</sub> for DMRG Wave Functions – Different Partitionings, Different Hamiltonians
Erik Hedegård	Dec. 1	First Explorations of DMRG with Polarizable Embedding
Christopher Stein	Dec. 8	Towards a Black-Box Multi-Reference Method: Single Molecules and Reactions
Alain Vaucher	Dec. 15	Real-Time Quantum Chemistry

<sup>a)</sup> Guest from the University of Strasbourg, France