

Special Topics in Theoretical Chemistry

Reiher Group Seminar (Tues. 2:30 pm, HCI G232)

Autumn Semester 2014

Seminar Rules

- Scheduled time for *group-member* talks: **20 min**
 - Scheduled time for *semester-student* talks: **10 min**
 - Before your talk: Employ LaTeX or PowerPoint templates for presentations available via [ETH CORPORATE COMMUNICATIONS](#)
 - During your talk: Tell what kind of software has been deposited where
 - After your talk: Upload your slides in both the original and PDF file format to the intranet
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Name	Date	Topic
Markus Reiher	Sept. 23	How to write a paper
Christopher Stein ^a	Oct. 8 2:00 pm	<i>Guest talk</i>
Arseny Kovyrshin	Oct. 14	Tensor Network Parametrization
Erik Hedegård	Oct. 21	Advances with DMRG and the Polarizable Embedding scheme
Tamara Husch ^b	Oct. 27 10:00 am	<i>Guest talk</i>
Halua Pinto de Magalhaes	Oct. 28	Generalized Orbital Transformations for the Application in Domain Averaged Fermi Holes
Yingjin Ma (1) Adrian Mühlbach ^c (2)	Nov. 4	Approximate gradients in state-averaged DMRG-SCF & tentative DMRG study on Ln/An complex (1) Analysis of theoretical models for the description of H ₂ activation by [Fe] hydrogenase (2)
Sebastian Keller	Nov. 11	Implementation of non-Abelian spin symmetry in Maquis
Maike Bergeler	Nov. 18	Towards an Automated QC Study of Chemical Mechanisms
Stefan Knecht	Nov. 25	Multireference Perturbation Theory for a DMRG Wavefunction – News and Views
Martin Stiebritz (1) Oliver Sala (2)	Dec. 2	A protein-design approach to study the reactivity of metalloenzymes (1) Kinetics and activation parameters of the trifluoromethylation reaction (2)
Florian Krausbeck (1) Philipp Zimmermann ^d (2)	Dec. 9	Progress in the Automatization of Gradient-Driven Molecule Construction (1) Vanadium-assisted trifluoromethylation of silyl ketene imines (2)
Jonny Proppe	Dec. 16	How predictive is theoretical ⁵⁷ Fe Mössbauer spectroscopy these days?

^aAlumnus of the University of Göttingen, Germany

^bAlumnus of the University of Ulm, Germany

^cSemester student of Arndt Finkelmann

^dSemester student of Oliver Sala