

Special Topics in Theoretical Chemistry

Autumn Semester 2019
Tuesday, 02:30 *p.m.* in HCI G 232

Speaker	Date	Title
Markus Reiher	Sep. 17	How to Write a Paper ¹
Stefan Gugler	Sep. 24	Gaussian Process-Based Refinement of Dispersion Corrections
Adrian Mühlbach	Oct. 01	SSUB for trajectories
Jan-Grimo Sobez	Oct. 08	Final advancements and thoughts on molassemble
Francesco Bosia	Oct. 15	Algorithmic Acceleration of Quantum Chemistry for an Interactive Experience
Alberto Baiardi	Oct. 22	Electron Dynamics with TD-DMRG
Christoph Brunken	Nov. 05	Automated Parametrization of System-Focused Atomistic Models for Nanoscale Systems by a Fragmentation-Based Approach
Stephanie Grimmel	Nov. 26	Predicting Chemical Reactivity from Distorted Structures
Vera von Burg	Dec. 10	Short-Range DFT: Progress and Challenges
Nina Glaser	Dec. 17	A study of FCIQMC
Yorrick Lassmann	Dec. 17	Systematic Basis Set Comparison in Molecular Systems and the Solid State
Severin Polonius	Dec. 17	Semiempirical electronic spectroscopy: beyond orthogonalization-corrected methods
Lucien Wernli	Dec. 17	Implementation and testing of the AFIR method within the Readuct framework

¹This talk is exclusively for Ph.D. and postdoctoral students of the Reiher Research group.