

Special Topics in Theoretical Chemistry

Reiher Group Seminar • FS 2016

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

Name	Date	Title
Markus Reiher	Feb. 23	How to Write a Paper
Jonny Proppe		Dimensionality Reduction of Markovian Networks
Gregor Simm	Mar. 1	Bayesian Error Estimation for Density Functionals
Vera von Burg	Mar. 15	How to Not Look at Orbital Pictures: Automated Orbital Active Space Selection for Metallocenes
Yingjin Ma		Progress of DMRG Derivative Techniques
Andrea Muolo	Apr. 5	Advances in Pre-Born–Oppenheimer Theory
Florian Krausbeck		Systematic Molecule Construction
Alain Vaucher	Apr. 19	Propensity Concepts in Real-Time Quantum Chemistry
Erik Hedegård	Apr. 26	DMRG with srDFT and Pair-DFT
Tamara Husch	May 10	Construction of Semi-Empirical Models
Arseny Kovyrshin	May 17	Update on Tensor Network Approaches
Leon Freitag	May 24	[Ru(bipy) ₃] ²⁺ Excitation Spectra