

Special Topics in Theoretical Chemistry

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

Speaker	Date	Title
Leon Freitag	Mar. 12	State-average DMRGSCF Gradients: A Light at the End of the Tunnel
Francesco Bosia, Jan Unsleber	Mar. 19	The New SCINE Software Architecture
Alberto Baiardi	Mar. 26	Time dependent density matrix renormalization group: from nuclear to electron dynamics
Vera von Burg	Apr. 02	In Search of a Satisfactory Solution to the Dynamic Correlation Problem
Arseny Kovyrshin	Apr. 09	Further developments in the CGTNS ansatz optimization
Christoph Brunken	Apr. 16	Self-Parametrizing System-Focused Molecular Models
Max Rossmannek	May 28	Natural Language Understanding for Quantum Chemical Calculations
Philipp Fischer	May 28	The Variational Monte Carlo optimization of the CGTNS ansatz
Robin Feldmann	May 28	Development of pre-Born–Oppenheimer Tensor Network algorithms
Stefan Knecht	June 18	Second-order orbital-optimisation with large-scale relativistic DMRG-SCF