Special Topics in Theoretical Chemistry

Spring Semester 2020
Tuesday, 02:30 *p.m.* in HCI G 232

Speaker	Date	Title
Thomas Weymuth	18.02.2020	Error Archigenesis with a Simple and Automated Incremental Scheme
Charlotte Müller	25.02.2020	Localization of Kohn-Sham Orbitals via Pivoted QR Decomposition
Max Mörchen	10.03.2020	Investigation of the Tailored Coupled Cluster Approach
Lina Eckert	17.03.2020	Quantum Mechanical Investigation of Napthalene Dioxygenase
Francesco Bosia	24.03.2020	Real-Time Spectroscopy with SCINE: First Results
Paul Türtscher	31.03.2020	Current Status of Automated Solvation with SCINE
Katja-Sophia Csizi	07.04.2020	A DFT study of oxygen activation in the active site of Naphthalene 1,2-Dioxygenase
Vera von Burg	21.04.2020	Analysis of electron correlation in short-range DFT
Christoph Brunken	28.04.2020	Implementation of hybrid quantum-mechanical / molecular-mechanical models into SCINE
Jan Unsleber	05.05.2020	Current Status of Automated Reaction Network Exploration with SCINE
Alberto Baiardi	12.05.2020	Electron and nuclear dynamics with TD-DMRG
Stefan Gugler	19.05.2020	Benchmarking and analysis of chemical reaction networks
Anna Kelemen	26.05.2020	Efficient anharmonic vibrational structure calculations with VDMRG-SCF
Severin Polonius	26.05.2020	Parametrization of semiempirical Hamiltonians for excited states