Special Topics in Theoretical Chemistry

Autumn Semester 2020
Tuesday, 02:45 – 03:30 *p.m.* in HCI G 3

Speaker	Date	Title
Michal Lesiuk	29.09.2020	Implementation of the Coupled-Cluster Method with Single, Double, and Triple Excitations using Tensor Decompositions
Thomas Weymuth	06.10.2020	Resonance Effects in the Raman Optical Activity Spectrum of $[Rh(en)_3]^{3+}$
Max Mörchen	13.10.2020	Reliability of Tailored Coupled Cluster in Different Correlation Regimes
Miguel Steiner	20.10.2020	Automated exploration of reaction mechanisms on surfaces
Alberto Baiardi	27.10.2020	Transcorrelated Density Matrix Renormalization Group
Stefan Gugler	03.11.2020	Bayesian Approach Toward Parametrized Physical Models
Paul Türtscher	10.11.2020	Iodine in Water: First Steps in Silico and Experimentally
Katja-Sophia Csizi	17.11.2020	Selective protein splicing to yield beta-amino acid residues via tyrosine excision
Stephanie Grimmel	24.11.2020	First-Principles Heuristics for Automated Reaction Space Exploration with Chemoton
Vera von Burg	01.12.2020	Quantum computing enhanced computational catalysis
Francesco Bosia	08.12.2020	Spectroscopy with semiempirical Hamiltonians