Special Topics in Theoretical Chemistry

Autumn Semester 2021
Tuesday, 01:45 – 02:30 *p.m.*, HCI G 7 (unless stated otherwise)

Talks on semester, bachelor and master theses should take about 10 minutes.
All other talks should be about 20 minutes in length.

Speaker	Date	Title
Paul Türtscher	28.09.2021	Pathfinder — A Route Planner for Chemical Reaction Networks
Robin Feldmann	05.10.2021	Nuclear-Electronic All-Particle Density Matrix Renormalization Group
Miguel Steiner	12.10.2021	Ahead of Density Functional Theory: Fantastic Semi-empirics and Where to Find Them
Alberto Baiardi	26.10.2021	Towards Massively Parallel DMRG with QCMaquis
Charlotte Müller	02.11.2021	Real-Time Haptic Quantum Chemistry: First User Study Results
Nina Glaser	09.11.2021	The Effect of Different Parametrizations on Vibrational Calculations in the Context of vDMRG
Stephanie Grimmel	16.11.2021	Chemoton 2.0 — Which Reactions Can We Find Now?
Max Mörchen	23.11.2021	Transcorrelated Coupled Cluster Theory
Jan Unsleber	30.11.2021	Current Advances in the SCINE Software Framework
Stefan Gugler	07.12.2021	Molecular Descriptors Rooted in Physical Principles for Machine-learning Energies
Katja-Sophia Csizi	14.12.2021	Automated Structure Preparation for QM/MM: pH-consistent Protonation of Biomolecules
Elizaveta Likhacheva	21.12.2021	Exploring the basis of homochirality: A Chemoton investigation of the Soai reaction
Umay Yildirim	21.12.2021	Testing Chemoton Using an Amine-Carboxylic Acid Coupling Map
Markus Fasching	21.12.2021	The Role of the Substrate in Dioxygen Activation by Rieske Non-Heme Dioxygenases
Enric Petrus Pérez	21.12.2021	Kinetic insights in the self-assembly of molybdenum and tungsten polyoxometalates