

Special Topics in Theoretical Chemistry

Spring Semester 2021
Tuesday, 02:45 – 03:30 *p.m.* via Zoom

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
Thomas Weymuth	02.03.2021	A Short Guide to the Reiher Research Group
Linh Tran	09.03.2021	Scale Factors and their Uncertainties for Fundamental Vibrational Frequencies
Jan Unsleber	16.03.2021	SCINE: An Update on the Current State of the Framework
Katja-Sophia Csizi	23.03.2021	Graph-Based Processing of Protein Structures: Sequence Analysis, Error Detection and Protonation
Paul Türtscher	13.04.2021	Iodine in Water: Exploration on Different Levels
Stefan Gugler	20.04.2021	Statistical Learning Theory for Combinatorial Density Functional Fitting
Michal Lesiuk	27.04.2021	Recent Progress in Transcorrelated and Rank-Reduced Density-Matrix Renormalization Group
Miguel Steiner	04.05.2021	Transferring Chemoton from gas phase to heterogeneous systems
Alberto Baiardi	11.05.2021	Excited-State Targeting Made Simple: The DMRG[FEAST] Approach
Max Mörchen	18.05.2021	Spin-Adapted Calculation of High-Order Density Matrices in DMRG
Charlotte Müller	25.05.2021	SCINE Interactive Update and How to Use It in Education
Veronika Klasovita	01.06.2021	tba
Chung Sum Leung	01.06.2021	tba
Moritz Baumgarten	01.06.2021	Limitations of Benchmarkings