

# Special Topics in Theoretical Chemistry

Spring Semester 2023

Tuesday, 01:45–02:30 *p.m.*, HCI J 3 (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
Miguel Steiner	21.02.2023	Spin multiplicity in automated reaction network explorations
Thomas Weymuth	07.03.2023	Quantum Phase Estimation
Nina Glaser	21.03.2023	Challenging FEAST: large-scale excited-state DMRG calculations
Moritz Bensberg	16.05.2023	Targeted Elementary Step Refinement through Sensitivity Analysis.
Katja Raue	30.05.2023	Disinfection of drinking water with chlorine—a mechanistical study
Valentin Barandun	30.05.2023	Large-Scale Quantum Dynamics of Excitons with TD-DMRG
Paul Fischill	30.05.2023	Towards large scale transcorrelated DMRG
Joel Landis	30.05.2023	Elimination of rotational motion from the pre-Born–Oppenheimer Hamiltonian