

Special Topics in Theoretical Chemistry

Autumn Semester 2023

Tuesday, 01:45–02:30 *p.m.*, HCI G 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
Markus Reiher	19.09.2023, HCI G 232	rETHink Discussion
Marco Eckhoff	03.10.2023	Lifelong Machine Learning Potentials
Mihael Erakovic	24.10.2023	Quantum Optimal Control with the Density Matrix Renormalization Group
Veronika Klasovita	31.10.2023	Towards accurately calculating electronically excited states with fast semiempirical methods
Francisco Fernandez Villoria	07.11.2023, HCI G 232	Few-fs Electron Transfer Dynamics in Photoionized Donor-Acceptor Molecules
Miguel Steiner	21.11.2023	Steering Wars: The Surface Strikes Back
Kalman Szenes	28.11.2023	Redesigning QCMAquis with performance in mind
Paul Türtscher	05.12.2023	A Chemical Reaction Network of the Bray-Liebhafsky Reaction
Jakob Assan	19.12.2023	Quantum Tunnelling Effects in Automated Chemical Network Explorations
Alberte Høholdt	19.12.2023	Disinfection of Drinking Water with Chlorine—analysis of exploration and results
Lea Hauswirth	19.12.2023	Reaction network exploration and method comparison for the formose reaction
Ramon Hügli	19.12.2023	A Mechanistic Study on the Soai Reaction via a Kinetically-Driven Chemical Reaction Network Exploration
Livia Hunkeler	19.12.2023	Automated Reaction Exploration of Tetramethylethene Ozonation
Timothy Stroschein	19.12.2023	Spectral analysis of large scale quantum systems through Prolate Filter Diagonalization and time dependent DMRG