

Special Topics in Theoretical Chemistry

Spring Semester 2024

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
Raphael Husistein	12.03.2024	Towards Growing Neural Networks for Lifelong Machine Learning Potentials
Valentin Barandun	19.03.2024	DMRG for Quantum Dynamics of Vibronic Systems with a new DMRG Lattice Mapping
Kalman Szenes	26.03.2024	Capturing electronic correlation using Jastrow factors
Guests	09.04.2024	tbd
Moritz Bensberg	07.05.2024	Astrochemistry with Chemoton
Veronika Klasovita	14.05.2024	Recent Additions to Sparrow
Robin Feldmann	21.05.2024	New Approaches to the Static–Dynamic Correlation Problem
Livia Hunkeler	28.05.2024	Improvements on Automated Reaction Search Algorithms
Daniel Isler	28.05.2024	Atomic Property Prediction by Lifelong Machine Learning
Carl Sünderhauf	28.05.2024	Zink-hemiacetalates as Autocatalysts — A Kinetically-Driven Chemical Reaction Network Exploration of the Soai Reaction
Matthias Kamm	28.05.2024	Adiabatic Excited State Preparation
