

# Special Topics in Theoretical Chemistry

Spring Semester 2022

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
n/a	22.02.2022	rETHink Discussion
Elena Jahr	01.03.2022	Dynamical Correlation in DMRG with the Adiabatic Connection
Moritz Bensberg	22.03.2022	Concentration Flux-Steered Exploration of One-Pot Chemistry
Paul Türtcher	05.04.2022	Towards an <i>ab Initio</i> Based Model of the Bray–Liebhafsky Reaction
Max Mörchen	26.04.2022	Recent Progress in Transcorrelated Coupled Cluster
Robin Feldmann	03.05.2022	The Trust-Region Augmented Hessian Method for (Nuclear-Electronic) Hartree–Fock
Miguel Steiner	10.05.2022	Investigating Catalysis with Chemoton
Veronika Klasovita	17.05.2022, 12:30	Theoretical Spectra of Porphyrin Systems
Stephanie Grimmel	31.05.2022	Reactivity Prediction from Chemoton Results

Please note also the following talks:

- Charlotte Müller, *Learning Chemical Concepts from Haptic Feedback: A Qualitative Study*, Future Learning Initiative Colloquium, 25.02.2022, 16:15, via Zoom<sup>1</sup>

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<sup>1</sup>Please register beforehand by writing to sara.may@gess.ethz.ch.