

Special Topics in Theoretical Chemistry

Autumn Semester 2022

Tuesday, 01:45–02:30 *p.m.*, HCI G 7 (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 (Place)	Title
Nina Glaser	27.09.2022 (HCI G 232)	Towards Large-Scale on-the-Fly vDMRG Calculations
Jan P. Unsleber	04.10.2022 (HCI G 232)	Automated Reaction Templating: ART (or Science?)
Veronika Klasovita	08.11.2022	An Introduction to MRCI
Robin Feldmann	15.11.2022	Towards Symmetry Projected Hartree–Fock
Moritz Bensberg	22.11.2022	Orbital Mapping
Marco Eckhoff	06.12.2022	Theoretical Investigation of Lithium Manganese Oxides Using High-Dimensional Neural Networks