

Special Topics in Theoretical Chemistry

Autumn Semester 2018

Speaker	Date	Title	Time and Place
Adrian Mühlbach	Oct. 16	Quantum System Partitioning at the Single-Particle Level	02:30 p.m., HCI G 232
Dr. Adam Kubas	Oct. 23	Unique ligation of [Fe ₄ S ₄] clusters: consequences for hydrogenases	02:30 p.m., HCI H 8.1
Prof. Markus Reiher	Oct. 30	How to Write a Paper	02:30 p.m., HCI G 232
Dr. Susi Lehtola	Nov. 6	Basis set limit Hartree-Fock and density functional theory calculations on atoms and diatomic molecules via finite elements	02:30 p.m., HCI G 232
Jan-Grimo Sobez	Nov. 13	Construction of a Universal Molecular Library	02:30 p.m., HCI G 232
Dr. Leon Freitag	Nov. 20	State-Averaged DMRG Gradients	02:30 p.m., HCI G 232
Dr. Arseny Kovyrshin	Nov. 27	Symmetry-Adapted Tensor Network States	02:30 p.m., HCI G 232
Annina Lieberherr	Dec. 4	Optimizing vDMRG With Quantum Entanglement	01:45 p.m., HCI G 232
Arian Kehrein	Dec. 4	Exploring Transition Metal Ligand Design	01:45 p.m., HCI G 232
Rhiannon Zarotiadis	Dec. 18	Property calculations from DMRG simulations	02:30 p.m., HCI G 232
Max Rossmannek	Dec. 18	Literature Seminar	02:30 p.m., HCI G 232