ETH *zürich*

Special Topics in Theoretical Chemistry

Reiher Group Seminar • HS 2017

Tuesday | 2:30 p.m. | HCI G 232/234

Name	Date	Title
Vera von Burg	10 Oct.	Automated Exploration of Complex Chemical Reaction Networks
Adrian H. Mühlbach	17 Oct.	Block-Diagonalization Embedding
Leon Freitag	31 Oct.	State-Average Density-Matrix-Renormalization-Group Self-Consistent-Field Gradients
Jan-Grimo Sobez	7 Nov.	Essential and Accidental Complexity in a Molecular Library
Tamara Husch	14 Nov.	Acceleration of Small-Basis-Set Hartree–Fock Calculations
Gregor N. Simm	28 Nov.	Error Estimation in Reaction Networks Through Gaussian Processes

as of 27 September 2017 | all information is subject to change