

Theoretisch-Chemisches Kolloquium (SS 2024)

Zeit: mittwochs 14:15, Ort: Seminarraum NC 5/99

10. 04. 2024	Thomas Gasevic , Mulliken Center for Theoretical Chemistry, Universität Bonn <i>Comprehensive Computational Studies of NMR Chemical Shifts for Group 14 Elements</i> (Seminarar Austauschprogramm Bonn/Bochum)
17. 04. 2024	Michal Kochmann , Institute of Physical Chemistry, Polish Academy of Sciences <i>Theory meets ultrafast spectroscopy: photophysics of donor-acceptor compounds</i> (Gemeinsames Seminar mit EXC 2033 „RESOLV“)
Sondertermin 24. 04. 2024 14:15, ZEMOS 0.17/0.19	Chiara Cappelli , Scuola Normale Superiore, Pisa, Italy <i>Multiscale Modeling of Spectroscopy in Complex Environments</i> (Gemeinsames Seminar mit EXC 2033 „RESOLV“)
08. 05. 2024	Motoyuki Shiga , Japan Atomic Energy Agency <i>Recent progress in ab initio path integral molecular dynamics</i> (Gemeinsames Seminar mit EXC 2033 „RESOLV“)
15. 05. 2024 abgesagt	Christoph Jacob , Theoretische Chemie, TU Braunschweig <i>Quantum-Chemical Calculation of Two-Dimensional Infrared Spectra</i> (Gemeinsames Seminar mit EXC 2033 „RESOLV“)
29. 05. 2024	Lukas Stelzl , Institute of Physics, JGU Mainz <i>Specific recognition and regulation by phase-separated condensates of disordered proteins: a simulations perspective</i> (Gemeinsames Seminar mit EXC 2033 „RESOLV“)
12. 06. 2024	Harald Oberhofer , Theoretische Physik IV, Universität Bayreuth <i>Simulating Charge Transport from First Principles to Machine Learning</i> (Gemeinsames Seminar mit EXC 2033 „RESOLV“)
19. 06. 2024	Stefan Goedecker , Department of Physics and Astronomy, University of Basel, Switzerland <i>Exploring the potential energy surface with Minima Hopping to study the synthesizability of materials</i> (Gemeinsames Seminar mit EXC 2033 „RESOLV“)
26. 06. 2024	Paul Popelier , Computational and Theoretical Chemistry, University of Manchester, UK <i>FFLUX or How to spend years constructing a novel force field based on Quantum Topological Atoms</i> (Gemeinsames Seminar mit EXC 2033 „RESOLV“)
03. 07. 2024	Tucker Carrington , Department of Chemistry, Queen's University, Ontario, Canada

Using collocation to solve the vibrational Schroedinger equation without computing integrals

(Gemeinsames Seminar mit EXC 2033 „RESOLV“)

10. 07. 2024

Andreas Grüneis, Technische Universität Wien

Recent developments in applying periodic coupled cluster theory to condensed matter systems

(Gemeinsames Seminar mit EXC 2033 „RESOLV“)

gez. Die Dozenten der Theoretischen Chemie

Gäste sind herzlich willkommen!