

Theoretisch-Chemisches Kolloquium (WS 2024/2025)

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

16. 10. 2024 **Sebastian Blach**, Theoretical Chemistry, Ruhr-Universität Bochum
Beneath the Surface: Decoding Methanol's hidden H-Bond Architecture
- Abgesagt**
13. 11. 2024 **Dr. Mira Todorova**, Department Computational Materials Design,
Electrochemistry and Corrosion Science, Max-Planck-Institut für Nachhaltige
Materialien Düsseldorf
TBA
- Special date**
20. 11. 2024 **Professor Johannes Margraf**, Physical Chemistry V: Theory and Machine
Learning, Universität Bayreuth
ZEMOS 0.17/0.19 *Extrapolating with Chemical Machine Learning*
(Gemeinsames Seminar mit EXC 2033 „RESOLV“)
27. 11. 2024 **Dr. David Wilkins**, School of Mathematics and Physics, Queen's University
Belfast
Machine Learning and Surface Vibrational Spectroscopy
04. 12. 2024 **Professor Bettina G. Keller**, Physical and Theoretical Chemistry, Freie
Universität Berlin
*Across molecular timescales: dynamical reweighting approaches to chemical
kinetics*
(Gemeinsames Seminar mit EXC 2033 „RESOLV“)
11. 12. 2024 **Professor Georg Kastlunger**, Department of Physics, Technical University
of Denmark
TBA
18. 12. 2024 **Johannes Gorges**, Theoretical Chemistry, Universität Bonn
*Quantum chemical calculation of mass spectra via automated reaction
network exploration*
(Seminar austauschprogramm Bonn/Bochum)
15. 01. 2025 **Professor Markus Reiher**, Institute for Molecular Physical Science,
Department of Chemistry and Applied Bioscience, ETH Zürich
*Automated and interactive quantum chemistry for reaction mechanism
elucidation*
22. 01. 2025 **Professor Andreas Köhn**, Institute for Theoretical Chemistry, Universität
Stuttgart
Coupled-cluster theory for multiconfigurational states - are we there yet
29. 01. 2025 **Professor Carl Caleman**, Department of Physics and Astronomy, X-ray
Photon Science, Uppsala University, Sweden
TBA

gez. Die Dozenten der Theoretischen Chemie

Gäste sind herzlich willkommen!