RUHR-UNIVERSITÄT BOCHUM

Lehrstuhl für Theoretische Chemie

RUB

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 **ZEMOS 0.17/0.19**	**Professor Johannes Margraf**, Physical Chemistry V: Theory and Machine Learning, Universität Bayreuth *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 *Non-Nernstian effects in electrocatalysis: How to simulate them and their consequences in mechanistic analyses*
18. 12. 2024	**Johannes Gorges**, Theoretical Chemistry, Universität Bonn *Quantum chemical calculation of mass spectra via automated reaction network exploration* (Seminaraustauschprogramm 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*
Abgesagt 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 *Modeling the dynamics and structure of matter exposed to ultrafast x-ray lasers with hybrid collisional-radiative/molecular dynamics*

gez. Die Dozenten der Theoretischen Chemie

Gäste sind herzlich willkommen!