

## Theoretical Chemistry Colloquia (WS 2024/2025)

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Time: Wednesdays 14:15, Location: Seminarraum NC 5/99

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16. 10. 2024      **Sebastian Blach**, Theoretical Chemistry, Ruhr-Universität Bochum  
*Beneath the Surface: Decoding Methanol's hidden H-Bond Architecture*
- Cancelled**  
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*  
(Joint seminar with 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*  
(Joint seminar with 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*  
(Speaker Exchange Program 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*
- Cancelled**  
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

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**Guests are most welcome!**