

Theoretical Chemistry Colloquia (SS 2025)

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

16. 04. 2025 **Professor Stephan Schlemmer**, Universität zu Köln, I. Physikalisches Institut
Missing ions in laboratory and in space
(Joint seminar with EXC 2033 “RESOLV”)
30. 04. 2025 **Professor Mira Todorova**, Max Planck Institute for Sustainable Materials, Düsseldorf
Potential dynamics and reactions at electrochemical interfaces studied by ab initio supercell calculations
(Joint seminar with EXC 2033 “RESOLV”)
07. 05. 2025 **Dr. Ulrich Meier**, IQM Quantum Computers, München
The Basis Concepts of Quantum Computing
(Joint seminar with EXC 2033 “RESOLV”)
14. 05. 2025 **Professor Felipe Fantuzzi**, University of Kent, School of Chemistry and Forensic Science, United Kingdom
From Chemical Bonds to Interstellar Space: Contributions from Theory
(Joint seminar with EXC 2033 “RESOLV”)
21. 05. 2025 **Professor Jagannath Mondal**, Tata Institute of Fundamental Research, Hyderabad, Indien
Generative machine learning approach in biomolecular Simulation
(Joint seminar with EXC 2033 “RESOLV”)
04. 06. 2025 **Professor Andreas Köhn**, Universität Stuttgart, Theoretische Chemie, Stuttgart
Coupled-cluster theory for multiconfigurational states - are we there yet?
18. 06. 2025 **Dr. Dorothea Golze**, Technische Universität Dresden, Computational Chemistry and Physics
TBA
(Joint seminar with EXC 2033 “RESOLV”)
25. 06. 2025 **Professor Shirin Faraji**, Heinrich Heine-Universität Düsseldorf, Theoretische Chemie und Computerchemie, Düsseldorf
Databased accelerated on-the-fly hybrid quantum/classical
(Joint seminar with EXC 2033 “RESOLV”)
09. 07. 2025 **Professor Patrick Rinke**, Technische Universität München, School of Natural Sciences, München
Machine-learning accelerated catalyst discovery and characterization
(Joint seminar with EXC 2033 “RESOLV”)
16. 07. 2025 **Marvin Friede**, Universität Bonn Mulliken Center for Theoretical Chemistry, Bonn
dxtb an efficient and fully differentiable framework for extended tight-binding
(Speaker Exchange Program Bonn/Bochum)

gez. Die Dozenten der Theoretischen Chemie

Guests are most welcome!