

Theoretical Chemistry Colloquia (SS 2025)

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

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

gez. Die Dozenten der Theoretischen Chemie

Guests are most welcome!