

Center for Theoretical Chemistry

Theoretical Chemistry Colloquia (WS 2025/2026)

Time: Wednesdays 14:15, Location: lecture hall NC 5/99

29. 10. 2025 **Tim Schramm**, Mulliken Center for Theoretical Chemistry, Universität Bonn
A 100.000-fold increase in C-H Bond Acidity gives Palladium a Key Advantage in C (sp³)-H Activation Compared to Nickel
(Speaker Exchange Program Bonn/Bochum)
05. 11. 2025 **Professor Christoph Jacob**, Institut für Physikalische und Theoretische Chemie, Technische Universität Braunschweig
Quantum-Chemical Calculation of 2D-IR Spectra
(Joint seminar with EXC 2033 “RESOLV”)
12. 11. 2025 **Professor Benjamin Fingerhut**, Department Chemie, Ludwig-Maximilians-Universität München
Excited state dynamics of biomolecular systems in complex environments
(Joint seminar with EXC 2033 “RESOLV”)
19. 11. 2025 **Professor Elke Pahl**, University of Auckland, New Zealand
Extreme(s) Matter: Alien Melting Behaviour of Noble Gases
(Joint seminar with EXC 2033 “RESOLV”)
17. 12. 2025 **Professor Guido Falk von Rudorff**, Computational Chemistry of Nanomaterials, Universität Kassel
Alchemical Perturbations and Machine Learning
(Joint seminar with EXC 2033 “RESOLV”)
07. 01. 2026 **Professor Ricardo Mata**, Computational Chemistry and Biochemistry Group, Georg-August Universität Göttingen
Nuclear quantum effects - the advent of multicomponent methods and benchmarks
(Joint seminar with EXC 2033 “RESOLV”)
- Special date**
14. 01. 2026 **ZEMOS 0.17/0.19** **Professor Peter Schreiner**, Institute of Organic Chemistry, Justus Liebig University Gießen
Rethinking Chemistry: the Role of Quantum Mechanical Tunneling
(Joint seminar with EXC 2033 “RESOLV”)
21. 01. 2026 **Professor Claudia Filippi**, Faculty of Science and Technology, University of Twente, Netherlands
Bridging accuracy and efficiency: Quantum Monte Carlo as a reference for machine learning
(Joint seminar with EXC 2033 “RESOLV”)
28. 01. 2026 **Professor Thomas Markland**, Stanford University, California, USA
Leveraging theory and simulation to decode and design multidimensional spectroscopies in the condensed phase
(Joint seminar with EXC 2033 “RESOLV”)

04.02.2026

Dr. Fabian Schuhmann, Niels Bohr Institute, Copenhagen, Denmark
TS2CG and Allostery: Building and Analyzing Lipid Membranes with Proteins
(Joint seminar with EXC 2033 “RESOLV”)

gez. Die Dozenten der Theoretischen Chemie

Guests are most welcome!