

## Theoretical Chemistry Colloquia (SS 2024)

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

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10. 04. 2024      **Thomas Gasevic**, Mulliken Center for Theoretical Chemistry, Universität Bonn  
*Comprehensive Computational Studies of NMR Chemical Shifts for Group 14 Elements*  
(Speaker Exchange Program Bonn/Bochum)
17. 04. 2024      **Michal Kochmann**, Institute of Physical Chemistry, Polish Academy of Sciences  
*Theory meets ultrafast spectroscopy: photophysics of donor-acceptor compounds*  
(Joint seminar with EXC 2033 “RESOLV”)
- Special date**  
24. 04. 2024      **Chiara Cappelli**, Scuola Normale Superiore, Pisa, Italy  
*Multiscale Modeling of Spectroscopy in Complex Environments*  
(Joint seminar with EXC 2033 “RESOLV”)  
**14:15, ZEMOS**
- 0.17/0.19**  
08. 05. 2024      **Motoyuki Shiga**, Japan Atomic Energy Agency  
*Recent progress in ab initio path integral molecular dynamics*  
(Joint seminar with EXC 2033 “RESOLV”)
- ~~15. 05. 2024~~      ~~**Christoph Jacob**, Theoretische Chemie, TU Braunschweig~~  
~~*Quantum-Chemical Calculation of Two-Dimensional Infrared Spectra*~~  
~~(Joint seminar with EXC 2033 “RESOLV”)~~  
**cancelled**
29. 05. 2024      **Lukas Stelzl**, Institute of Physics, JGU Mainz  
*Specific recognition and regulation by phase-separated condensates of disordered proteins: a simulations perspective*  
(Joint seminar with EXC 2033 “RESOLV”)
12. 06. 2024      **Harald Oberhofer**, Theoretische Physik IV, Universität Bayreuth  
*Simulating Charge Transport from First Principles to Machine Learning*  
(Joint seminar with EXC 2033 “RESOLV”)
19. 06. 2024      **Stefan Goedecker**, Department of Physics and Astronomy, University of Basel, Switzerland  
*Exploring the potential energy surface with Minima Hopping to study the synthesizability of materials*  
(Joint seminar with EXC 2033 “RESOLV”)
26. 06. 2024      **Paul Popelier**, Computational and Theoretical Chemistry, University of Manchester, UK  
*FFLUX or How to spend years constructing a novel force field based on Quantum Topological Atoms*  
(Joint seminar with EXC 2033 “RESOLV”)
03. 07. 2024      **Tucker Carrington**, Department of Chemistry, Queen’s University, Ontario, Canada

*Using collocation to solve the vibrational Schroedinger equation without computing integrals*

(Joint seminar with EXC 2033 “RESOLV”)

10.07.2024

**Andreas Grüneis**, Technische Universität Wien

*Recent developments in applying periodic coupled cluster theory to condensed matter systems*

(Joint seminar with EXC 2033 “RESOLV”)

gez. Die Dozenten der Theoretischen Chemie

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**Guests are most welcome!**