

## Theoretical Chemistry Colloquia (SS 2023)

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

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19. 04. 2023      **Florian Bischoff**, Institut für Chemie, Humboldt Universität zu Berlin  
*Computing molecular properties in real space*
26. 04. 2023      **Robert Meißner**, Molekulardynamische Simulation weicher Materie,  
Technische Universität Hamburg  
*TBA*  
(Joint seminar with EXC 2033 “RESOLV”)
03. 05. 2023      **Florian Weigend**, Applied Quantum Chemistry, Philipps-Universität Marburg  
*Relativity in quantum chemistry: recent developments and applications*  
(Joint seminar with EXC 2033 “RESOLV”)
10. 05. 2023      **Roberto Covino**, FIAS - Frankfurt Institute of Advanced Studies  
*Investigating mechanisms of biomolecular self-organization by integrating  
physics-based simulations and AI*  
(Joint seminar with EXC 2033 “RESOLV”)
17. 05. 2023      **A. Marco Saitta**, Institut de Minéralogie, de Physique des Matériaux et de  
Cosmochimie (IMPMC), Université Pierre et Marie Curie - Sorbonne, France  
*Ab initio and machine learning approaches to prebiotic chemistry/origins of  
life studies*  
(Joint seminar with EXC 2033 “RESOLV”)
24. 05. 2023      **Thomas Heine**, Lehrstuhl für Theoretische Chemie, Technische Universität  
Dresden  
*Mattermorphosis*  
(Joint seminar with EXC 2033 “RESOLV”)
07. 06. 2023      **Michael Schmitt**, Institut für Physikalische Chemie,  
Heinrich-Heine-Universität Düsseldorf  
*Molecules in their electronically excited states - Modulation of structures, life  
times and dipole moments*
14. 06. 2023      **Daan Geerke**, Molecular and Computational Toxicology, Vrije Universiteit  
Amsterdam, Netherlands  
*Deriving a Polarizable Force Field for Biomolecules with Minimal Empirical  
Calibration*  
(Joint seminar with EXC 2033 “RESOLV”)
21. 06. 2023      **Uwe Manthe**, Theoretische Chemie, Universität Bielefeld  
*Quantum dynamics of reactions and fluid motions*  
(Joint seminar with EXC 2033 “RESOLV”)
28. 06. 2023      **Amalendu Chandra**, Theoretical Chemistry Group, Indian Institute of  
Technology, India  
*Nonlinear vibrational spectroscopy of aqueous systems: Use of spectral maps  
and beyond*  
(Joint seminar with EXC 2033 “RESOLV”)

12. 07. 2023

**Thomas Froitzheim**, Mulliken Center for Theoretical Chemistry, Universität Bonn

*Method, Structure and Embedding: What TADF Emitters can teach us about Quantum Chemistry*

(Speaker Exchange Program Bonn/Bochum)

gez. Die Dozenten der Theoretischen Chemie

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**Guests are most welcome!**