

Theoretical Chemistry Colloquia (WS 2023/2024)

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

11. 10. 2023 **Sandipan Mohanty**, Jülich Supercomputing Centre, Forschungszentrum Jülich
Quantum annealing: some applications in biophysics
 (Joint seminar with EXC 2033 “RESOLV”)
- Special date**
 18. 10. 2023
ZEMOS 0.17/0.19 **Pascal Friederich**, Artificial Intelligence for Materials Science, Department of Informatics and Institute of Nanotechnology, Karlsruhe Institute of Technology
Machine Learning for Simulation, Understanding, and Design of Molecules and Materials
 (Joint seminar with EXC 2033 “RESOLV”)
25. 10. 2023 **Benedikt Bädorf**, Theoretical Chemistry, Universität Bonn
Efficient Computation of Very Large, Non-covalently Bound Complexes
 (Speaker Exchange Program Bonn/Bochum)
08. 11. 2023 **Frank Ortmann**, Theoretical Methods in Spectroscopy, TUM School of Natural Sciences, Technische Universität München
Excitations in Energy Materials: Insights from Theory
 (Joint seminar with EXC 2033 “RESOLV”)
15. 11. 2023 **Christoph Jacob**, Institut für Physikalische und Theoretische Chemie, Technische Universität Braunschweig
Quantum-Chemical Calculation of Two-Dimensional Infrared Spectra
 (Joint seminar with EXC 2033 “RESOLV”)
06. 12. 2023 **Matthias Rupp**, Luxembourg Institute of Science and Technology (LIST)
Selection, validation, and application of machine-learning potentials at the examples of thermal transport and a phase transition in dense hydrogen
 (Joint seminar with EXC 2033 “RESOLV”)
13. 12. 2023 **Sascha Jähnigen**, Université PSL, Sorbonne Université and CNRS
Periodic calculations of vibrational circular dichroism: How is it supposed to work?
 (Joint seminar with EXC 2033 “RESOLV”)
- Special date**
 18. 01. 2024
15:15, ZEMOS 0.17/0.19 **Gregor Jung**, Biophysikalische Chemie, Universität des Saarlandes
Photoacids - a unique combination of photochemistry and fluorescence
 (Joint seminar with EXC 2033 “RESOLV”)

gez. Die Dozenten der Theoretischen Chemie

Guests are most welcome!