RUHR-UNIVERSITÄT BOCHUM

# Center for Theoretical Chemistry

RUB

## Theoretical Chemistry Colloquia (WS 2022/2023)

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

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| **ZEMOS 0.17**<br>14. 09. 2022 | **Christoph Schran**, Department of Chemistry, University of Cambridge, United Kingdom<br>*Understanding complex aqueous systems with machine learning*<br>(Joint seminar with EXC 2033 "RESOLV") |
| 19. 10. 2022 | **Shota Tsuru**, Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum<br>*Sampling and modeling for spectral simulation for solution systems*<br>(Joint seminar with EXC 2033 "RESOLV") |
| 26. 10. 2022 | **Florian Pabst**, Napolitano Laboratory, Polymer and Soft Matter Dynamics, Université libre de Bruxelles, Belgium<br>*Dielectric and light scattering spectra - Their differences and how to understand them*<br>(Joint seminar with EXC 2033 "RESOLV") |
| 09. 11. 2022 | **Christof Holzer**, Karlsruher Institut für Technologie<br>*From Molecules to Optical Materials using GPUs: Advances in Quantum Chemical Methods* |
| 16. 11. 2022 | **Daniel Sebastiani**, Institut für Chemie - Theoretische Chemie, Martin-Luther-Universität Halle-Wittenberg<br>*Simulation of Proton Mobility in Condensed Phases at large scales and with near quantum chemical accuracy*<br>(Joint seminar with EXC 2033 "RESOLV") |
| 23. 11. 2022 | **Hilke Bahmann**, Bergische Universität Wuppertal<br>*Flexible hybrid density functionals for electronic interfaces* |
| 30. 11. 2022 | **Christoph Plett**, Mulliken Center for Theoretical Chemistry, Rheinische Friedrich-Wilhelms-Universität Bonn<br>*Modeling Explicit Solvation with the Quantum Cluster Growth Algorithm*<br>(Joint seminar with EXC 2033 "RESOLV")<br>(Speaker Exchange Program Bonn/Bochum) |
| 07. 12. 2022 | **Thomas Kühne**, Dynamics of Condensed Matter, University of Paderborn<br>*Novel Electronic Structure Methods to Break the Exaflop Barrier*<br>(Joint seminar with EXC 2033 "RESOLV") |
| 14. 12. 2022 | **Meinard Kuhlmann**, Philosophisches Seminar, Johannes-Gutenberg-Universität Mainz<br>*The quantum measurement problem - A critical discussion of competing solutions* |

gez. Die Dozenten der Theoretischen Chemie

**Guests are most welcome!**