

Theoretical Chemistry Colloquia (WS 2019/2020)

Time: Wednesdays 14:15, Location: Seminarraum NC 03/399

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| Special date | Sonia Coriani , Department of Chemistry, University of Denmark, Copenhagen, Denmark |
| Thu 10. 10. 2019 | |
| 15:00, ZEMOS 0.17 | <i>Theoretical 'Beamlines' for Modern Spectroscopic Experiments</i>
(Joint seminar with EXC 2033 "RESOLV") |
| 23. 10. 2019 | Michael Walter , Freiburg Centre for Interactive Materials and Bioinspired Technologies, University of Freiburg
<i>From bond rupture to weakly interacting systems - insights from density functional theory</i> |
| 30. 10. 2019 | Oldamur Hollóczki , Mulliken Center for Theoretical Chemistry, Institut für Physikalische und Theoretische Chemie, Universität Bonn
<i>Nanoplastics from molecular dynamics simulations</i>
(Speaker Exchange Program Bonn/Bochum) |
| 06. 11. 2019 | Mihkel Ugandi , Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum
<i>Exploration of excited state potential energy surfaces: computations and implementation</i> |
| 13. 11. 2019 | Laura Durán Caballero , Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum
<i>Quantum solvation of Molecules in para-hydrogen</i> |
| 20. 11. 2019 | Reinhold Fink , Institut für Physikalische und Theoretische Chemie, Universität Tübingen
<i>Approaching chemical accuracy with second order perturbation theory by mixing RE and MP Hamiltonians and orbital optimization</i> |
| 27. 11. 2019 | Benjamin Rotenberg , Laboratoire PHENIX, Sorbonne Université, Paris, France
<i>Electrode/electrolyte interfaces: insights from classical molecular simulations and applications to energy storage, blue energy harvesting and water desalination</i>
(Joint seminar with EXC 2033 "RESOLV") |
| 04. 12. 2019 | Esma Birsan Boydas , Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum
<i>Mechanistic insights into the reduction of carbon dioxide by supramolecular mixed-valent complexes from quantum chemical calculations</i> |
| 18. 12. 2019 | Klaus-Robert Müller , Institute of Software Engineering and Theoretical Computer Science, Machine Learning, Technische Universität Berlin
<i>Machine Learning meets Quantum Chemistry</i>
(Joint seminar with EXC 2033 "RESOLV") |

- 08.01.2020 **Ivano Tavernelli**, IBM Zurich Research Laboratory, Zürich, Schweiz
Quantum computing and its applications in chemistry and physics
(Joint seminar with EXC 2033 “RESOLV”)
- 15.01.2020 **Toon Verstraelen**, Center for Molecular Modeling, Techlane Ghent Science Park, Campus Ardoyen, Zwijnaarde, Belgien
Force Field Modeling of Short-Range Induction Interactions and Polarizable Atomic Monopoles
(Joint seminar with EXC 2033 “RESOLV”)
- 22.01.2020 **Samuli Ollila**, Institute of Biotechnology, University of Helsinki, Finland
Combination of NMR Experiments and MD Simulations to Study Disordered Biomolecules
(Joint seminar with EXC 2033 “RESOLV”)
- 29.01.2020 **Birgit Strodel**, Forschungszentrum Jülich, Biophysics and Soft Matter, Jülich
Possibilities and current limitations of joining MD simulations and experiments
(Joint seminar with EXC 2033 “RESOLV”)
- Special date**
Wed 05.02.2020
14:15 **Sapna Sarupria**, Chemical and Biomolecular Engineering, Clemson University, USA
Pushing the limits of simulations of complex systems – from nucleation to biomolecules, from rare event sampling to multiscale modeling
(Joint seminar with EXC 2033 “RESOLV” and “Research Department Solvation Science”)

gez. Die Dozenten der Theoretischen Chemie

Guests are most welcome!