

Lehrstuhl für Theoretische Chemie

Ruhr-Universität Bochum

www.theochem.ruhr-uni-bochum.de

Theoretical Chemistry Colloquia (WS 2017/2018)

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

- Special date** **Teresa Head-Gordon**, University of California at Berkeley, USA
We 25. 10. 2017 *Water and Binary Systems under Confinement*
14:15, ZEMOS 0.17 (Joint seminar with EXC 1069 "RESOLV")
- Special date** **Martin Head-Gordon**, University of California at Berkeley, USA
Mo 30. 10. 2017 *Modeling electrocatalytic reduction of CO₂ on copper electrodes*
15:15, ZEMOS 0.17 (Joint seminar with EXC 1069 "RESOLV")
- Special date** **Sarah Khani**, Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum
Th 02. 11. 2017 *Solvent Effects on Halogen-bonded Ion Pairs*
15. 11. 2017 **Vera Krewald**, University of Bath, Department of Chemistry, UK
Electronic structure analysis of transition metal dimers for dinitrogen photocleavage
29. 11. 2017 **Till Rudack**, Lehrstuhl für Biophysik, Ruhr-Universität Bochum
From Atom to Cell: MD Simulation Techniques to Bridge Computation and Experiment
06. 12. 2017 **Oldamur Hollóczki**, Mulliken Center for Theoretical Chemistry, Universität Bonn
On the Role of Carbenes in N-Heterocyclic Carbene Organocatalysis
(Speaker Exchange Program Bonn / Bochum)
13. 12. 2017 **Sebastian Höfener**, Karlsruhe Institute of Technology, Institute of Physical Chemistry, Karlsruhe
Computing UV/vis spectra of solvated molecules using frozen-density embedding methods
-CANCELLED-
(Joint seminar with EXC 1069 "RESOLV")
20. 12. 2017 **Gunnar Schmitz**, Department of Chemistry, Aarhus University, Denmark
Data reduction in Quantum Chemistry: Applying more general mathematical tools
10. 01. 2018 **Tristan Berau**, Max Planck Institute for Polymer Research, Mainz
Augmenting multiscale simulations by data-driven methods
(Joint seminar with EXC 1069 "RESOLV")
24. 01. 2018 **Simon Bernèche**, Computational Sciences, University of Basel, Switzerland
Exploring novel molecular mechanisms in biological channels and transporters using free energy simulations
(Joint seminar with EXC 1069 "RESOLV")
31. 01. 2018 **Carsten Baldauf**, Theoretische Chemie, Fritz-Haber-Institut Berlin, Max-Planck-Gesellschaft
Biomolecules in Thin Air
(Joint seminar with EXC 1069 "RESOLV")

gez. Die Dozenten der Theoretischen Chemie

Visitors are welcome to the seminar.