Lehrstuhl für Theoretische Chemie

Ruhr-Universität Bochum

www.theochem.ruhr-uni-bochum.de

Theoretisch-Chemisches Kolloquium (WS 2017/2018)

Zeit: mittwochs 14:15, Ort: Seminarraum NC 03/399

Sondertermin **We 25.** 10. 2017 14:15, ZEMOS 0.17	**Teresa Head-Gordon**, University of California at Berkeley, USA *Water and Binary Systems under Confinement* (Gemeinsames Seminar mit EXC 1069 "RESOLV")
Sondertermin **Mo 30.** 10. 2017 15:15, ZEMOS 0.17	**Martin Head-Gordon**, University of California at Berkeley, USA *Modeling electrocatalytic reduction of CO2 on copper electrodes* (Gemeinsames Seminar mit EXC 1069 "RESOLV")
Sondertermin **Do 02.** 11. 2017	**Sarah Khani**, Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum *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* (Seminaraustauschprogramm 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-*** (Gemeinsames Seminar mit 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 Bereau**, Max Planck Institute for Polymer Research, Mainz *Augmenting multiscale simulations by data-driven methods* (Gemeinsames Seminar mit 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* (Gemeinsames Seminar mit EXC 1069 "RESOLV")
31. 01. 2018	**Carsten Baldauf**, Theoretische Chemie, Fritz-Haber-Institut Berlin, Max-Planck-Gesellschaft *Biomolecules in Thin Air* (Gemeinsames Seminar mit EXC 1069 "RESOLV")

gez. Die Dozenten der Theoretischen Chemie

Gäste sind herzlich willkommen !