

Lehrstuhl für Theoretische Chemie

Ruhr-Universität Bochum

www.theochem.ruhr-uni-bochum.de

Theoretisch-Chemisches Kolloquium (SS 2017)

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

19. 04. 2017 **Knut Asmis**, Theoretische Chemie, Wilhelm-Ostwald-Institut, Universität Leipzig
Spectroscopic Snapshots of the Proton Transfer Mechanism in Water
(Gemeinsames Seminar mit EXC 1069 "RESOLV")
26. 04. 2017 **Heike Fliegl**, Centre for Theoretical and Computational Chemistry, Oslo University, Norway
Calculations of magnetically induced currents: theory and applications
03. 05. 2017 **Allan East**, Department of Chemistry and Biochemistry, University of Regina, Canada
Modelling Solvated Systems: Possible Improvement of the Continuum Dielectric Model
(Gemeinsames Seminar mit EXC 1069 "RESOLV")
31. 05. 2017 **Fabio Sterpone**, Laboratoire de Biochimie Théorique, Institut de Biologie Physico-Chimique, Paris, France
Toward microscopic simulations of the cellular environment
(Gemeinsames Seminar mit EXC 1069 "RESOLV")
- Sondertermin** **Ondrej Marsalek**, Department of Chemistry, Stanford University, USA
Fr 09. 06. 2017 *Quantum dynamics and spectroscopy of ab initio aqueous solutions: the interplay of nuclear and electronic quantum effects*
(Gemeinsames Seminar mit EXC 1069 "RESOLV")
14. 06. 2017 **Benjamin Helmich-Paris**, Amsterdam Institute for Molecules, Medicines and Systems, Freie Universität Amsterdam, Niederlande
Towards an accurate computational electronic spectroscopy of large heavy-element containing molecules: Exploring a Laplace-transformed atomic and active molecular orbital formulation of relativistic and multireference perturbation theories
21. 06. 2017 **Sandro Jahn**, Institut für Geologie und Mineralogie, Universität zu Köln
Molecular scale modeling of geological melts and fluids
(Gemeinsames Seminar mit EXC 1069 "RESOLV")
28. 06. 2017 **Alfons Geiger**, Physikalische Chemie, Technische Universität Dortmund
Microscopic Structure and Unusual Properties of Water
(Gemeinsames Seminar mit EXC 1069 "RESOLV")
12. 07. 2017 **Jakob Seibert**, Mulliken Center for Theoretical Chemistry, Rheinische Friedrich-Wilhelms-Universität Bonn
xTB -- A robust and versatile tight-binding package
(Seminar austauschprogramm Bonn / Bochum)
26. 07. 2017 **Alireza Marefat Khah**, Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum
Molecular Gradients of Polarizable Embedded RI-CC2: Seeking to Understand the Excited-State Pathways of Berenil

gez. Die Dozenten der Theoretischen Chemie

Gäste sind herzlich willkommen !