Lehrstuhl für Theoretische Chemie

Ruhr-Universität Bochum

www.theochem.ruhr-uni-bochum.de

Theoretical Chemistry Colloquia (SS 2017)

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

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19. 04. 2017	**Knut Asmis**, Theoretische Chemie, Wilhelm-Ostwald-Institut, Universität Leipzig *Spectroscopic Snapshots of the Proton Transfer Mechanism in Water* (Joint seminar with 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* (Joint seminar with 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* (Joint seminar with EXC 1069 "RESOLV")
Special date **Fr 09.** 06. 2017	**Ondrej Marsalek**, Department of Chemistry, Stanford University, USA *Quantum dynamics and spectroscopy of ab initio aqueous solutions: the interplay of nuclear and electronic quantum effects* (Joint seminar with 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* (Joint seminar with EXC 1069 "RESOLV")
28. 06. 2017	**Alfons Geiger**, Physikalische Chemie, Technische Universität Dortmund *Microscopic Structure and Unusual Properties of Water* (Joint seminar with 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* (Speaker Exchange Program 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

Visitors are welcome to the seminar.