Lehrstuhl für Theoretische Chemie

Ruhr-Universität Bochum

www.theochem.ruhr-uni-bochum.de

Theoretical Chemistry Colloquia (SS 2016)

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

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13. 04. 2016 **David Tew**, School of Chemistry, University of Bristol, United Kingdom
Quantum dynamics on accurate electronic potentials

27. 04. 2016 **Markus Reiher**, Laboratory of Physical Chemistry, ETH Zürich, Switzerland
Second Generation Density Matrix Renormalization Group

04. 05. 2016 **Stephan Gekle**, Theoretische Physik, Universität Bayreuth
Interaction of light and fluids: from microwaves to organic solar cells
(Joint seminar with EXC 1069 "RESOLV")

11. 05. 2016 **Jens Smiatek**, Institute for Computational Physics, University of Stuttgart
Coarse-grained simulations of macromolecules: The influence of physical and chemical effects
(Joint seminar with EXC 1069 "RESOLV")

25. 05. 2016 **Nora Graf**, Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum
Analytic second derivatives for excited state with RI-CC2

01. 06. 2016 **Robin Santra**, Center for Free-Electron Laser Science, DESY, Department of Physics, University of Hamburg
Extreme states of matter: From terahertz- to x-ray-driven dynamics
(Joint seminar with EXC 1069 "RESOLV")

08. 06. 2016 **Sebastian Dohm**, Mulliken Center for Theoretical Chemistry, Universität Bonn
Creating QM-derived Force Fields with fragmented Hessians
(Speaker Exchange Program Bonn / Bochum)

15. 06. 2016 **Mauro Boero**, IPCMS Œ Département de Chimie et des Matériaux Inorganiques (DCMI), CNRS-University of Strasbourg, France
Solvation Properties of Metal Alkali Ions and Role of van der Waals Interactions
(Joint seminar with EXC 1069 "RESOLV")

22. 06. 2016 **Jörg Kussmann**, Lehrstuhl für Theoretische Chemie, Ludwig-Maximilian-Unversität München
Quantum Chemistry on Graphics Processing Units (GPU)

29. 06. 2016 **Vlad Cojocaru**, Computational Structural Biology Laboratory, Max Planck Institute for Molecular Biomedicine, Münster
Mechanisms of cooperativity in protein-DNA binding from atomistic simulations

06. 07. 2016 **Sandeep Sharma**, Max-Planck-Institute for Solid Research, Stuttgart
Chemical applications and theory of matrix product states

13. 07. 2016 **Bettina Keller**, Department of Biology, Chemistry, Pharmacy Institute of Chemistry and Biochemistry, Freie Universität Berlin
Kinetic models for intrinsically disordered peptides from molecular dynamics simulations
(Joint seminar with EXC 1069 "RESOLV")

20. 07. 2016 **Marius Frank**, Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum
PNO-MP2 and its application to molecular geometries and first order properties

gez. Die Dozenten der Theoretischen Chemie

Visitors are welcome to the seminar.