

Lehrstuhl für Theoretische Chemie

Ruhr-Universität Bochum

www.theochem.ruhr-uni-bochum.de

Theoretisch-Chemisches Kolloquium (SS 2014)

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

16. 04. 2014 **Michael Römel**, Department of Chemistry, Princeton University
N-Electron Valence Perturbation Theory for DMRG-Wavefunctions
30. 04. 2014 **Péter Szalay**, Laboratory of Theoretical Chemistry, Institute of Chemistry, Eötvös Loránd University, Budapest
Can Coupled-Cluster Methods Be Used to Describe Excited States of the Building Blocks of DNA?
07. 05. 2014 **Dirk Möhlmann**, Deutsches Zentrum für Luft- und Raumfahrt e.V., Berlin
Water on Mars
-CANCELLED-
(Gemeinsames Seminar mit EXC 1069 "RESOLV")
- Sondertermin Do 08.** 05. 2014 **Gerhard Hummer**, Abteilung Theoretische Biophysik, Max-Planck-Institut für Biophysik, Frankfurt
17:15, HNC 30 *Molecular simulation of protein dynamics and function*
14. 05. 2014 **Ricardo Mata**, Computational Chemistry and Biochemistry Group, Georg-August-Universität, Göttingen
A hierarchy of embedding approaches for computational studies in solution
(Gemeinsames Seminar mit EXC 1069 "RESOLV")
04. 06. 2014 **Oliver Kühn**, Institute of Physics, University of Rostock
Raum: NC 5/99 *Theoretical X-ray Spectroscopy of Transition Metals in Solution*
(Gemeinsames Seminar mit EXC 1069 "RESOLV")
18. 06. 2014 **Christoph Reimann**, Mulliken Center for Theoretical Chemistry, Universität Bonn
Electronic and Thermodynamic Properties of Metastable Vanadium Oxides
02. 07. 2014 **Jan Urban**, Department of Biophysics and Chemical Physics, Comenius University, Bratislava
Fragmentation of Negative Ions: Theoretical Description
09. 07. 2014 **Julien Michel**, School of Chemistry, University of Edinburgh
Exploring biomolecular hydration thermodynamics with grid cell theory
(Gemeinsames Seminar mit EXC 1069 "RESOLV")
16. 07. 2014 **Christian Lennartz**, Teamleader Modelling Organic Electronics, BASF SE, Ludwigshafen
Organic Electronics: From Molecules to Devices

gez. Die Dozenten der Theoretischen Chemie

Gäste sind herzlich willkommen !