

# Lehrstuhl für Theoretische Chemie

## Ruhr-Universität Bochum

www.theochem.ruhr-uni-bochum.de

### Theoretical Chemistry Colloquia (SS 2014)

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

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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-**  
(Joint seminar with EXC 1069 "RESOLV")
- Special date** **Gerhard Hummer**, Abteilung Theoretische Biophysik, Max-Planck-Institut für  
**Th 08.** 05. 2014 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*  
(Joint seminar with EXC 1069 "RESOLV")
04. 06. 2014 **Oliver Kühn**, Institute of Physics, University of Rostock  
**Room: NC 5/99** *Theoretical X-ray Spectroscopy of Transition Metals in Solution*  
(Joint seminar with 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*  
(Joint seminar with 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

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**Visitors are welcome to the seminar.**