

Lehrstuhl für Theoretische Chemie

Ruhr-Universität Bochum

www.theochem.ruhr-uni-bochum.de

Theoretical Chemistry Colloquia (SS 2011)

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

06. 04. 2011 **Tobias Schwabe**, Department of Chemistry, Faculty of Science, Aarhus University
The Polarizable Embedding Approach for QM/MM Systems: Theoretical Background and Application
13. 04. 2011 **Eberhard K. U. Gross**, Theory Department, Max Planck Institute of Microstructure Physics, Halle (Saale)
How to make the Born-Oppenheimer approximation exact: A fresh look on potential energy surfaces and Berry phases
20. 04. 2011 **Paul Popelier**, School of Chemistry, University of Manchester, United Kingdom
Polarisation in force fields: time for a step change?
27. 04. 2011 no colloquium
04. 05. 2011 **Vincenzo Barone**, Scuola Normale Superiore, Pisa
Computational Spectroscopy: from small molecules to nano systems
(Joint seminar with FOR 618 "Aggregation")
11. 05. 2011 **Ben Feringa**, Stratingh Institute for Chemistry, University of Groningen
In control of molecular motion - from switches to motors
(Reinhard Koselleck Lecture)
18. 05. 2011 **Thomas Müller**, Jülich Supercomputing Centre, Forschungszentrum Jülich
Recent developments of the COLUMBUS ab-initio program package
25. 05. 2011 **Daniel Kats**, Institut für Physikalische und Theoretische Chemie, Universität Regensburg
Low scaling methods for excited states
01. 06. 2011 **Robert Iszak**, Theoretische Chemie, Rheinische Friedrich-Wilhelms Universität Bonn
An Overlap Fitted RIJCOSX Theory
(Speaker Exchange Program Bonn / Bochum)
08. 06. 2011 **Irene Burghardt**, Departement de chimie, Ecole Normale Supérieure, Paris
Quantum Dynamics of Photoprocesses in Extended Molecular Systems: Coherence and Dissipation at the Nanoscale
(Joint seminar with FOR 618 "Aggregation")
15. 06. 2011 no colloquium
- Special date** **Thorsten Klüner**, Theoretische Chemie, Carl von Ossietzki Universität, Oldenburg
Tu 21. 06. 2011
11:15, NC 2/99 *Quantum Dynamics on Surfaces: A Theoretical Perspective*
(Joint seminar with SFB 558 "Heterogeneous Catalysis")
- Special date** **Christian Ochsenfeld**, Theoretische Chemie, Ludwig-Maximilians-Universität München
Th 30. 06. 2011
17:00, HNC 30 *Intermolecular Interaction in Molecular Systems with 1000 and More Atoms - Challenges for Quantum Chemistry*
(General Colloquia of the Department)
06. 07. 2011 **Damien Laage**, Chemistry Department, Ecole Normale Supérieure, Paris
Room: NC 2/99 *Theory and Simulation of Solvation in Aqueous Solutions*
(Joint seminar with FOR 618 "Aggregation")
- Special date** **Christopher Handley**, Department of Chemistry, University of Warwick
Th 11. 08. 2011
Time: 10:15 *Machine Learning: Novel Approaches to Force Field Representation and Parametrization*
- Special date** **Ilja Siepmann**, Department of Chemistry, University of Minnesota, USA
Th 29. 09. 2011
16:15, NC 03/399 *Simulation Studies of Hydrogen-bonding Systems: Structure, Solvation, and Phase Equilibria*
(Joint seminar with FOR 618 "Aggregation")

gez. Die Dozenten der Theoretischen Chemie

Visitors are welcome to the seminar.