Lehrstuhl für Theoretische Chemie

Ruhr-Universität Bochum

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Theoretisch-Chemisches Kolloquium (SS 2011)

Zeit: mittwochs 14:15, Ort: 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	kein Kolloquium
04. 05. 2011	**Vincenzo Barone**, Scuola Normale Superiore, Pisa *Computational Spectroscopy: from small molecules to nano systems* (Gemeinsames Seminar mit 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 Vorlesung)
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* (Seminaraustauschprogramm Bonn / Bochum)
08. 06. 2011	**Irene Burghardt**, Departement de chimie, Ecole Normale Superieure, Paris *Quantum Dynamics of Photoprocesses in Extended Molecular Systems: Coherence and Dissipation at the Nanoscale* (Gemeinsames Seminar mit FOR 618 "Aggregation")
15. 06. 2011	kein Kolloquium
Sondertermin **Di 21.** 06. 2011 11:15, **NC 2/99**	**Thorsten Klüner**, Theoretische Chemie, Carl von Ossietzki Universität, Oldenburg *Quantum Dynamics on Surfaces: A Theoretical Perspective* (Gemeinsames Seminar mit SFB 558 "Heterogene Katalyse")
Sondertermin **Do 30.** 06. 2011 17:00, **HNC 30**	**Christian Ochsenfeld**, Theoretische Chemie, Ludwig-Maximilians-Universität München *Intermolacular Interaction in Molecular Systems with 1000 and More Atoms - Challenges for Quantum Chemistry* (GDCh Kolloquium der Fakultät)
06. 07. 2011 **Raum: NC 2/99**	**Damien Laage**, Chemistry Department, Ecole Normale Superieure, Paris *Theory and Simulation of Solvation in Aqueous Solutions* (Gemeinsames Seminar mit FOR 618 "Aggregation")
Sondertermin **Do 11.** 08. 2011 **Zeit: 10:15**	**Christopher Handley**, Department of Chemistry, University of Warwick *Machine Learning: Novel Approaches to Force Field Representation and Parametrization*
Sondertermin **Do 29.** 09. 2011 **16:15**, NC 03/399	**Ilja Siepmann**, Department of Chemistry, University of Minnesota, USA *Simulation Studies of Hydrogen-bonding Systems: Structure, Solvation, and Phase Equilibria* (Gemeinsames Seminar mit FOR 618 "Aggregation")

gez. Die Dozenten der Theoretischen Chemie

Gäste sind herzlich willkommen !