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 RIJCOX Theory
(Speaker Exchange Program 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
(Joint seminar with FOR 618 “Aggregation”)

15. 06. 2011  no colloquium

Th 21. 06. 2011  Thorsten Klüner, Theoretische Chemie, Carl von Ossietzki Universität, Oldenburg
Quantum Dynamics on Surfaces: A Theoretical Perspective
(Joint seminar with SFB 558 “Heterogeneous Catalysis”)

Th 30. 06. 2011  Christian Ochsenfeld, Theoretische Chemie, Ludwig-Maximilians-Universität München
Intermolecular Interaction in Molecular Systems with 1000 and More Atoms - Challenges for Quantum Chemistry
(General Colloquium of the Department)

06. 07. 2011  Damien Laage, Chemistry Department, Ecole Normale Superieure, Paris
Theory and Simulation of Solvation in Aqueous Solutions
(Joint seminar with FOR 618 “Aggregation”)

Th 11. 08. 2011  Christopher Handley, Department of Chemistry, University of Warwick
Machine Learning: Novel Approaches to Force Field Representation and Parametrization

Th 29. 09. 2011  Ilja Siepmann, Department of Chemistry, University of Minnesota, USA
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.