

Lehrstuhl für Theoretische Chemie

Ruhr-Universität Bochum

www.theochem.ruhr-uni-bochum.de

Theoretical Chemistry Colloquia (WS 2011/2012)

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

19. 10. 2011 **Martin Müser**, Lehrstuhl für Materialsimulation, Universität des Saarlandes
From electronic DFT to continuum mechanics based descriptions of tribological phenomena
(Joint seminar with SFB 558 "Heterogeneous Catalysis")
26. 10. 2011 **Benjamin Helmich**, Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum
Local pair natural orbitals for excited states
- Special date** **Malgorzata Krasowska**, Faculty of Chemistry, University of Wroclaw, Poland
Th 27. 10. 2011 *Intramolecular hydrogen bonding in thiosemicarbazones and dipyrrens*
09. 11. 2011 **Hauke Clausen-Schaumann**, Physikalische Technik, Hochschule für Angewandte Wissenschaften, München
Chemical Reactions under Force: Kinetic Measurements of Mechanically Activated Bond Scission
(Reinhard Koselleck Vorlesung)
16. 11. 2011 **Christoph Jacob**, CFN-Nachwuchsgruppe Theoretische Chemie, Karlsruher Institut für Technologie
Subsystem and Embedding Methods for Quantum Chemistry
23. 11. 2011 **Tucker Carrington Jr.**, Chemistry Department, Queen's University, Ontario
Computing ro-vibrational spectra
14. 12. 2011 **Jean-Francois Lambert**, Laboratoire de Reactivite de Surface, Universite Pierre et Marie Curie, Paris
Small Biomolecules on Inorganic Oxide Surfaces; Adsorption Mechanisms, Reactivity, and Prebiotic Buildup of Complexity
(Joint seminar with SFB 558 "Heterogeneous Catalysis")
11. 01. 2012 **Gregor Diezemann**, Theoretische Chemie, Johannes Gutenberg-Universität Mainz
Force Probe Molecular Dynamics Simulations of Reversible Hydrogen-Bond Network Dynamics in Supramolecular Complexes
(Reinhard Koselleck Vorlesung)
18. 01. 2012 **Joachim Dzubiella**, Institut für Weiche Materie und Funktionale Materialien, Helmholtz-Zentrum Berlin
Modeling Hydration and Ion-Specific Effects in Protein Folding and Association
(Joint seminar with FOR 618 "Aggregation")
- Special date** **Axel Groß**, Institut für Theoretische Chemie, Universität Ulm
Tu 24. 01. 2012 *First Principles Description of Elementary Steps in Electrocatalysis*
11:15, NC 2/99 (Joint seminar with SFB 558 "Heterogeneous Catalysis")
01. 02. 2012 **Benoit Champagne**, Laboratoire de Chimie Theorique, Facultes Universitaires Notre-Dame de la Paix, Namur
Predicting and interpreting the second- and third-order nonlinear optical properties: from simple to more complex systems
14. 03. 2012 **Mark Tuckerman**, Department of Chemistry and Courant Institute, New York University
Exploring free energy landscapes of peptides, polymers, and molecular crystals
(Joint seminar with FOR 618 "Aggregation")
- Special date** **Toru Shiozaki**, Universität Stuttgart, Institut für Theoretische Chemie
Mo 26. 03. 2012 *Recent developments in multireference electronic structure theories*

gez. Die Dozenten der Theoretischen Chemie

Visitors are welcome to the seminar.