

Lehrstuhl für Theoretische Chemie

Ruhr-Universität Bochum

www.theochem.ruhr-uni-bochum.de

Theoretisch-Chemisches Kolloquium (WS 2008/2009)

Zeit: mittwochs 14:15, Ort: Seminarraum NC 03/399

22. 10. 2008 **Jutta Rogal**, Van 't Hoff Institute for Molecular Sciences, University of Amsterdam
Multiple State Transition Path Sampling
(Gemeinsames Seminar mit SFB 558 "Heterogene Katalyse")
29. 10. 2008 kein Kolloquium
05. 11. 2008 **John McCaskill**, Biomolecular Information Processing, BioMedizinZentrum
Dortmund
*Physical self-assembly and chemical reactions towards artificial cells: A tool for
systems chemistry*
12. 11. 2008 **Andreas Hansen**, Lehrstuhl für Theoretische Chemie, Universität Bonn
Efficient and accurate quantum chemical methods for large molecules
(Seminar austauschprogramm Bonn / Bochum)
19. 11. 2008 **Robert Berger**, Frankfurt Institute for Advanced Studies, Frankfurt am Main
Large-scale vibronic structure methods: Franck-Condon factors and beyond
26. 11. 2008 **Lynn Kamerlin**, Department of Chemistry, University of Southern California, Los
Angeles
Dineopentyl Phosphate Hydrolysis: Evidence for Stepwise Water Attack
03. 12. 2008 **Sabre Kais**, Department of Chemistry, Birck Nanotechnology Center, Purdue
University
Finite Size Scaling and Quantum Criticality
10. 12. 2008 **Teodoro Laino**, IBM Research Zurich
Long range interactions in semi-empirical NDDO Hamiltonians
17. 12. 2008 **Rosa Bulo**, Theoretical Chemistry, Free University of Amsterdam
Chemistry in Solution: Adaptive QM/MM Simulations
07. 01. 2009 **Johannes Frenzel**, Department of Chemistry, University of Calgary
*Does the surface matter? Aspects from theoretical investigations on metal,
semiconductor and oxide based nanomaterials*
14. 01. 2009 **José D. Faraldo-Gómez**, Max Planck Institute of Biophysics, Frankfurt am Main
*Thermodynamical analysis of biomolecular complexes through classical computer
simulations*
21. 01. 2009 **Joachim Friedrich**, Institut für Theoretische Chemie, Universität zu Köln
The Incremental Scheme - A Local Correlation Approach
- Sondertermin** **Georg Madson**, Department of Physics and Astronomy, University of Aarhus
Di 27. 01. 2009 *Au clusters on defected TiO₂ surfaces*
11:15, NC 5/99 (Gemeinsames Seminar mit SFB 558 "Heterogene Katalyse")
04. 02. 2009 **Guido Roßmüller**, Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum
*Embedded Cluster calculation on the ZnO-Catalyzed Synthesis of Methanol from CO
and H₂*

gez. Die Dozenten der Theoretischen Chemie

Gäste sind herzlich willkommen !