Lehrstuhl für Theoretische Chemie

Ruhr-Universität Bochum

www.theochem.ruhr-uni-bochum.de

Theoretical Chemistry Colloquia (WS 2008/2009)

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

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22. 10. 2008	**Jutta Rogal**, Van 't Hoff Institute for Molecular Sciences, University of Amsterdam *Multiple State Transition Path Sampling* (Joint seminar with SFB 558 "Heterogeneous Catalysis")
29. 10. 2008	no colloquium
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* (Speaker Exchange Program 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, Universtät zu Köln *The Incremental Scheme - A Local Correlation Approach*
Special date **Tu 27.** 01. 2009 11:15, NC 5/99	**Georg Madson**, Department of Physics and Astronomy, University of Aarhus *Au clusters on defected TiO_2 surfaces* (Joint seminar with SFB 558 "Heterogeneous Catalysis")
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 H_2*

gez. Die Dozenten der Theoretischen Chemie

Visitors are welcome to the seminar.