Lehrstuhl für Theoretische Chemie

Ruhr-Universität Bochum

www.theochem.ruhr-uni-bochum.de

Theoretical Chemistry Colloquia (WS 2009/2010)

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

Special date **Tu 13.** 10. 2009 11:15, NC 5/99	**Roman Martonak**, Department of Experimental Physics, Comenius University, Bratislava *Study of polymorphism and structural transformations in crystals by metadynamics simulation* (Joint seminar with SFB 558 "Heterogeneous Catalysis")
21. 10. 2009	**Ehesan Ali**, Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum *Tuning the Magnetic Coupling of Metalloporphyrin Molecules to Ferromagnetic Substrates*
28. 10. 2009	**Michael Hanrath**, Institut für Theoretische Chemie, Universität Köln *Multi-Reference Coupled Cluster: Perspectives, Theory, and Efficient Implementation*
04. 11. 2009	**Guntram Rauhut**, Institut für Theoretische Chemie, Universität Stuttgart *From the construction of accurate potential energy surfaces to the calculation of vibrational wavefunctions* (Joint seminar with SFB 558 "Heterogeneous Catalysis")
11. 11. 2009	**Rint Sijbesma**, Molecular Science and Technology, Eindhoven University of Technology *Chemistry Induced by Mechanical Force* (Reinhard Koselleck Lecture)
18. 11. 2009	**Martin Beyer**, Institut für Physikalische Chemie,Christian-Albrechts-Universität zu Kiel *Mechanochemistry - The Mechanical Activation of Covalent Bonds* (Reinhard Koselleck Lecture)
25. 11. 2009	**Jürgen Fritz**, School of Engineering and Science,Jacobs University Bremen *Imaging, Pulling, Bending: Atomic Force Microscopy on Biomolecular Systems* (Joint seminar with FOR 618 "Aggregation")
Special date **Tu 01.** 12. 2009 11:15, NC 5/99	**Thomas Heine**, Theoretical Physics, Jacobs University Bremen *Hydrogen Storage in Nanoporous Materials: Myths and Facts* (Joint seminar with SFB 558 "Heterogeneous Catalysis")
Special date **Tu 08.** 12. 2009	**Matteo Farnesi Camellone**, National Simulation Center, Trieste *Reaction Mechanisms for the CO Oxidation on Au/CeO2 Catalysts* (Joint seminar with SFB 558 "Heterogeneous Catalysis")
09. 12. 2009	**Rachel Glaves**, Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum *Understanding Enzymatic Reaction Mechanisms using QM/MM Simulations: Hydrolysis of Nucleotides in hGBP1*
16. 12. 2009	**Daniel Boese**, Theoretische Organische Chemie, Universität Duisburg-Essen *From Ab Inito Methods to the Development of New Force Fields*
23. 12. 2009	no colloquium
06. 01. 2010	no colloquium
13. 01. 2010	**Simone Koßmann**, Lehrstuhl für Theoretische Chemie, Universität Bonn *Improved Second Order Many-Body Perturbation Theory - Implementation and Validation* (Speaker Exchange Program Bonn / Bochum)
20. 01. 2010	**Markus Reiher**, Laboratorium für Physikalische Chemie, ETH Zürich *Quantum Chemical Methods for Vibrational Spectroscopy of Functional Molecules* (Joint seminar with SFB 558 "Heterogeneous Catalysis")
27. 01. 2010	**Hermann Kümmel**, Institut für Theoretische Physik, Ruhr-Universität Bochum *The Story of the Coupled Cluster Method*
03. 02. 2010	**Nongnuch Artrith**, Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum *High-Dimensional Neural Network Potentials: First Applications to Zinc Oxide*

gez. Die Dozenten der Theoretischen Chemie

Visitors are welcome to the seminar.