

Lehrstuhl für Theoretische Chemie

Ruhr-Universität Bochum

www.theochem.ruhr-uni-bochum.de

Theoretical Chemistry Colloquia (WS 2002/2003)

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

23. 10. 2002 **Karl Kleinermanns**, Institut für Physikalische Chemie und Elektrochemie, Heinrich-Heine-Universität, Düsseldorf
Laser Spectroscopy of isolated DNA bases and base pairs
30. 10. 2002 **Roman Kovacik**, Department of Biophysics and Chemical Physics, Comenius Universität, Bratislava
Modelling of the interaction of merocyanine-540 with a lipid bilayer
06. 11. 2002 **Padma Kumar P.**, Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum
Computer simulation studies of ionic motion in NASICON-type superionic conductors
13. 11. 2002 **Magali Benoit**, Laboratoire des Verres, Université Montpellier II
Structural and vibrational properties of silicate glasses from ab initio MD simulations
- Special date** **Xavier Gonze**, Unité de Physico-Chimie et de Physique des Matériaux (PCPM),
Tu 19. 11. 2002 Université catholique de Louvain, Belgium
11:15, NC 5/99 *DFT treatment of polarized systems and polar surfaces*
(Joint seminar with SFB 558 "Heterogeneous Catalysis")
27. 11. 2002 **Thomas Krüger**, Theoretische Physik, Universität Paderborn
Myth, horseplay or reality? The Einstein-Podolsky-Rosen-'Paradox' and its consequences
04. 12. 2002 **Beate Paulus**, MPI für Physik komplexer Systeme, Dresden
Ab initio incremental correlation treatment for metals
- Special date** **Georg Kresse**, Center for Computational Materials Science, Universität Wien
Tu 10. 12. 2002 *Novel Stabilization Mechanism on Polar Surfaces: ZnO (0001)-Zn*
11:15, NC 5/99 (Joint seminar with SFB 558 "Heterogeneous Catalysis")
18. 12. 2002 **Frank Großmann**, Institut für Theoretische Physik, Technische Universität Dresden
Conductance Calculations for Real Systems on the Nanoscale
08. 01. 2003 **Rajendra Prasad**, Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum
Laser induced desorption of CO from Cr₂O₃(0001)
15. 01. 2003 **Richard Dronskowski**, Institut für Anorganische Chemie, RWTH Aachen
Room: NC 5/99 *Itinerant Ferro- and Antiferromagnetism and Chemical Bonding*
(Joint seminar with Inorganic Chemistry)
22. 01. 2003 **Wim Klopper**, Institut für Physikalische Chemie, Universität Karlsruhe
Can R12 theory be successfully applied to large molecules?
29. 01. 2003 **Eduard Schreiner**, Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum
Conformation transitions in elastin models
(Joint seminar with FOR 436 "Water at Interfaces")
- Special date** **Ria Broer**, University of Groningen, Netherlands
Tu 04. 02. 2003 *Excitations and magnetic coupling in transition metal oxides*
11:15, NC 5/99 (Joint seminar with SFB 558 "Heterogeneous Catalysis")
12. 02. 2003 **Jürg Hutter**, Physikalisch Chemisches Institut, Universität Zürich
Excited state calculations with plane wave basis sets

gez. Die Dozenten der Theoretischen Chemie

Visitors are welcome to the seminar.