

Lehrstuhl für Theoretische Chemie

Ruhr-Universität Bochum

www.theochem.ruhr-uni-bochum.de

Theoretical Chemistry Colloquia (WS 2006/2007)

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

18. 10. 2006 no colloquium
25. 10. 2006 **Bernd Schimmelpfennig**, Institut für Nukleare Entsorgung, Forschungszentrum Karlsruhe
Computational actinide chemistry close to experiment
- Special date** **Jörg Neugebauer**, Computational Materials Design, Max-Planck-Institut für Eisenforschung Düsseldorf
- Tu 07. 11. 2006 11.15, NC 5/99 *Obtaining thermodynamic and kinetic properties of surfaces from first principles*
(Joint seminar with SFB 558 "Heterogeneous Catalysis")
- Special date** **Karsten Albe**, Institut für Materialwissenschaft, Technische Universität Darmstadt
- Tu 14. 11. 2006 11.15, NC 5/99 *Thermodynamics and kinetics of point defects in ZnO*
(Joint seminar with SFB 558 "Heterogeneous Catalysis")
- Special date** **Jörg Behler**, Computational Science, ETH USI-Campus, Lugano
- Mo 20. 11. 2006 *Metadynamics simulations of phase transitions in solids*
Time: 11.15
22. 11. 2006 **Peter Reinhardt**, Lab. Chimie Theorique, Universite Paris VI
Epstein-Nesbet perturbation theory is far from useless - if employed with localized orbitals
29. 11. 2006 **Erik T. J. Nibbering**, Max-Born-Institut für Nichtlineare Optik und Kurzzeitspektroskopie Berlin
Proton transfer dynamics in hydrogen bonded systems
(Joint seminar with FOR 618 "Aggregation")
06. 12. 2006 **Roman Kovacik**, Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum
Characterization of catalyst surfaces by STM image calculations
13. 12. 2006 **Teodor S. Balaban**, Institut für Nanotechnologie, Forschungszentrum Karlsruhe
Diastereotopic Ligation of Magnesium Atoms in (Bacterio)Chlorophylls
20. 12. 2006 **Günter von Kiedrowski**, Bioorganische und Supramolekulare Chemie, Ruhr-Universität Bochum
Systems chemistry - a way to tackle the origin-of-life problem a little better decoupled from scientific believes and religions
10. 01. 2007 **Arnim Hellweg**, Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum
Applications of the ricc2 program
17. 01. 2007 **Mike Gillan**, London Centre for Nanotechnology, University College London
First-principles modelling of nano-systems containing many thousands of atoms
(Joint seminar with SFB 558 "Heterogeneous Catalysis")
24. 01. 2007 **Eliseo Ruiz**, Department of Inorganic Chemistry, University of Barcelona
Single molecule magnets and other large magnetic polynuclear complexes: a theoretical study using density functional methods
31. 01. 2007 **Ove Christiansen**, Theoretical Chemistry Group, University of Aarhus
Vibrational structure theory
(Joint seminar with SFB 558 "Heterogeneous Catalysis")
07. 02. 2007 **Eduard Schreiner**, Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum
Iron-sulfur world: prebiotic chemistry

gez. Die Dozenten der Theoretischen Chemie

Visitors are welcome to the seminar.