Lehrstuhl für Theoretische Chemie

Ruhr-Universität Bochum

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Theoretical Chemistry Colloquia (WS 2003/2004)

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

15. 10. 2003	**Veronika Brazdova**, Institut für Chemie, Humboldt Universität Berlin *Periodic density functional calculations on vanadium oxide aggregates: structures, stability and vibrational spectra* (Joint seminar with SFB 558 "Heterogeneous Catalysis")
22. 10. 2003	**Per Jensen**, Theoretische Chemie, Universität Wuppertal *Molecular structure determination: quantum chemistry and spectroscopy vs. Coulomb explosion imaging for small molecules*
29. 10. 2003	**Stephan Thiel**, Max-Planck-Institut für Kohlenforschung, Mülheim an der Ruhr *QM/MM studies of the enzyme-catalysed aromatic hydroxylation of p-hydroxybenzoate*
05. 11. 2003	**Klaus Doll**, Institut für Mathematische Physik, TU Braunschweig *Ab initio calculations for metals with a local basis set*
Special date **Tu 11.** 11. 2003 11:15, NC 5/99	**Notker Rösch**, Theoretische Chemie, TU München *Metal clusters on oxide supports* (Joint seminar with SFB 558 "Heterogeneous Catalysis")
19. 11. 2003	**Martin Albrecht**, Theoretische Chemie, Universität Siegen *First-principle calculations of charge transport through single molecules*
26. 11. 2003	**Stefan Goedecker**, Institut für Physik, Universität Basel *Towards the virtual chemistry and physics laboratory* (Joint seminar with SFB 558 "Heterogeneous Catalysis")
03. 12. 2003	**Andreas Heßelmann**, Theoretische Organische Chemie, Universität Duisburg-Essen *A combined Kohn-Sham and intermolecular perturbation theory approach*
Special date 10. 12. 2003 **Time: 16:15**	**Martin Zacharias**, Computational Biology, International University Bremen *Computer simulation of biomolecule dynamics and complex formation* (Joint seminar with FOR 436 "Water at Interfaces")
Special date **Mo 15.** 12. 2003 **Time: 16:15**	**Dimitri Khoshtariya**, Institute of Molecular Biology and Biophysics, Georgian Academy of Sciences *Local hydrogen-bonded structures of water - from bulk to protein surface and the interior* (Joint seminar with FOR 436 "Water at Interfaces")
17. 12. 2003	**Ilka Hegemann**, Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum *Investigation of Cu/ZnO-catalysts - a cluster approach*
07. 01. 2004	**Michael Schmitt**, Physikalische Chemie, Universität Düsseldorf *Determination of the structure of large isolated molecules in various electronic states*
14. 01. 2004	**Tony Scott**, Theoretische Organische Chemie, Universität Duisburg-Essen *Asymtotics of quantum mechanical systems via the Holstein-Herring method*
Special date **Th 15.** 01. 2004 **Time: 13:15**	**Robert Zillich**, Department of Chemistry, University of California at Berkeley *Spectroscopy of molecules in superfluid helium-4 clusters*
21. 01. 2004	**Irmgard Frank**, Physikalische Chemie, LMU München *Simulation of ultrafast reactions with first-principles molecular dynamics*
28. 01. 2004	**Frank Neese**, Max-Planck-Institut für Bioanorganische Chemie, Mülheim an der Ruhr *Theoretical spectroscopy of open-shell transition metal complexes*
Special date **Th 29.** 01. 2004 **Time: 16:15**	**Rodolphe Pollet**, Laboratoire Francis Perrin, Saclay/Gif-sur-Yvette Cedex, France *Cooperative effects in a molecular dynamics simulation of a lanthanum(III)-water cluster*
04. 02. 2004	**Holger Langer**, Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum *Photophysics of guanine: a nonadiabatic Car-Parrinello study*

gez. Die Dozenten der Theoretischen Chemie

Visitors are welcome to the seminar.