Lehrstuhl für Theoretische Chemie

Ruhr-Universität Bochum

www.theochem.ruhr-uni-bochum.de

Theoretical Chemistry Colloquia (WS 2001/2002)

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

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24. 10. 2001	**Daniel Krüger**, Physikalisches Institut, Universität Münster *Simulation of the bond rupture process of thiolate on gold*
31. 10. 2001	**John Stubbs**, Department of Chemistry, University of Minnesota (currently at RUB) *Monte Carlo simulations for the aggregation of alkanols in nonpolar solvents*
07. 11. 2001	**Florian Müller-Plathe**, Max-Planck-Institut für Polymerforschung, Mainz *Simulating polymers on serveral length scales: Methods and applications*
Special date **Fr 09.** 11. 2001	**Daniel Boese**, Theoretical Chemistry, Cambridge University (currently at RUB) *Development and assessment of exchange-correlation functionals*
14. 11. 2001	no colloquium
21. 11. 2001	**Roger Rousseau**, Lehrstuhl für Theoretische Chemie, Universität Bochum *Phase stability and structural chemistry at high pressure*
28. 11. 2001	**Uwe Birkenheuer**, Max-Planck-Institut für Physik komplexer Systeme, Dresden *Ab initio determination of correlated wavefunctions for excited hole and electron capture states in solids*
05. 12. 2001	**Michael Rohlfing**, Institut für Festkörpertheorie, Universität Münster *Excited states and optical spectra of solids, surfaces and molecules*
Special date **Fr 14.** 12. 2001	**Rajendra Prasad**, Lehrstuhl für Theoretische Chemie, Universität Bochum *Ab initio studies of electronic structure and molecular properties of transient molecules in their ground and excited states*
19. 12. 2001 **seminar cancelled**	**W. H. Eugen Schwarz**, Theoretische Chemie, Universität Siegen *Single configuration DFT for states with strong configuration mixing?*
09. 01. 2002	**Gerald Geudtner**, Theoretische Chemie, Universität Hannover *Growth of Cu- and Ga-clusters on MgO*
Special date **Tu 15.** 01. 2002 11:15, NC 5/99	**Mike W. Finnis**, School of Mathematics and Physics, The Queen's University of Belfast *Theory of oxide-metal interfaces: structure and stoichiometry*
23. 01. 2002	**Christian Ochsenfeld**, Institut für Physikalische Chemie, Universität Mainz *Linear scaling in ab initio methods for large molecules*
30. 01. 2002	**Holger Langer**, Lehrstuhl für Theoretische Chemie, Universität Bochum *Ab initio study of excited states of DNA-bases and base pairs*
06. 02. 2002	**Reinhold Egger**, Theoretische Physik, Universität Düsseldorf *Real time path integral Monte Carlo Simulations*
13. 02. 2002	**Michael Atanasov**, Theoretische Chemie, Universität Düsseldorf *Theoretical studies of cyano complexes*

gez. Die Dozenten der Theoretischen Chemie

Visitors are welcome to the seminar.