Lehrstuhl für Theoretische Chemie

Ruhr-Universität Bochum

www.theochem.ruhr-uni-bochum.de

Theoretical Chemistry Colloquia (SS 2009)

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

---

22. 04. 2009	**Sebastian Höfener**, Institut für Physikalische Chemie, Lehrstuhl für Theoretische Chemie, Universität Karlsruhe *Time-independent properties from explicitly correlated methods*
29. 04. 2009	**Asbjörn Burow**, Lehrstuhl für Theoretische Chemie, Humboldt-Universität zu Berlin *Calculation of Coulomb energies for periodic systems with DFT, Gaussian basis functions, and the resolution of identity method* (Joint seminar with SFB 558 "Heterogeneous Catalysis")
Special date **Tu 05.** 05. 2009 11:15, NC 5/99	**Michael Springborg**, Physikalische und Theoretische Chemie, Universität des Saarlandes, Saarbrücken *Theoretical Studies of Structural and Electronic Properties of Clusters* (Joint seminar with SFB 558 "Heterogeneous Catalysis")
13. 05. 2009	**Jörg Koßmann**, Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum *Calculation of vibrational frequencies of adsorbates and adatoms on ZnO surfaces*
20. 05. 2009	**Johannes Kästner**, Institut für Theoretische Chemie, Universität Stuttgart *Biochemical Simulations using QM/MM Techniques*
27. 05. 2009	**Michael Römelt**, Lehrstuhl für Theoretische Chemie, Universität Bonn *EPR spectroscopic properties of Mo[(hiptN)$_3$NX], X=N$_2$, CO, NH$_3$* (Speaker Exchange Program Bonn / Bochum)
10. 06. 2009	**Daniel Borgis**, Laboratory for Analysis and Modelling for Biology and Environment, University of Evry-Val d'Essonne, Evry *Coarse-graining proteins and water for protein-protein interactions*
17. 06. 2009	**Sara Bonella**, Department of Physics, University of Rome *Trajectory based simulations of mixed quantum-classical time correlation functions* (Joint seminar with FOR 618 "Aggregation")
Special date **Tu 23.** 06. 2009 11:15, NC 5/99	**Thomas Bredow**, Lehrstuhl für Theoretische Chemie, Universität Bonn *Adsorption at metal and oxide surfaces: some challenges for theory* (Joint seminar with SFB 558 "Heterogeneous Catalysis")
01. 07. 2009	**Klaus Ruedenberg**, Department of Chemistry and Ames Laboratory, Iowa State University *Accurate potential energy curves and the transition from the covalent to the van der Waals regime*
08. 07. 2009	**Sonia Coriani**, Università degli Studi di Trieste, Trieste *In silico determination of spectroscopic properties: a few recent methodological and applicative results*
15. 07. 2009	**Bernd Ensing**, Van't Hoff Institute for Molecular Sciences, University of Amsterdam *Multiscale molecular dynamics of chemical and biophysical transitions*

gez. Die Dozenten der Theoretischen Chemie

Visitors are welcome to the seminar.