Lehrstuhl für Theoretische Chemie

Ruhr-Universität Bochum

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Theoretical Chemistry Colloquia (SS 2004)

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

Special date 21. 04. 2004 **Time: 11:15**	**Alexander Wolf**, Theoretische Chemie, Universität Bonn *Decoupling schemes for the Dirac Hamiltonian and the generalized Douglas-Kroll transformation* (Exchange seminar with Universität Bonn)
28. 04. 2004	**Thomas Elsässer**, Max-Born-Institut, Berlin *Ultrafast hydrogen bond dynamics and proton transfer in the liquid phase*
05. 05. 2004	**Pekka Pyykkö**, Department of Chemistry, University of Helsinki *QED-effects in chemistry*
12. 05. 2004	**Joachim Heberle**, Biologische Strukturforschung, Forschungszentrum Jülich *The vibrations of active proton transfer across the cell membrane* (Joint seminar with FOR 436 "Water at Interfaces")
19. 05. 2004	**Andreas Heyden**, Chemische Reaktionstechnik, Technische Universität Hamburg-Harburg *Determination of reaction paths for the dissociation of N_2O in Fe-ZSM5*
26. 05. 2004	**Fritz Haake**, Theoretische Physik, Universität Duisburg-Essen *Decoherence or why the world behaves classically*
02. 06. 2004	**Karin Fink**, Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum *Magnetic exchange coupling in transition metal compounds*
09. 06. 2004	**Werner Kutzelnigg**, Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum *The Nooijen conjecture: A detective story*
16. 06. 2004	**Jürgen König**, Theoretische Physik, Ruhr-Universität Bochum *Electron transport through interacting quantum dots*
23. 06. 2004	**Claudia Filippi**, Lorentz Institute for Theoretical Physics, Leiden University *Excitations in photoactive molecules from quantum Monte Carlo*
30. 06. 2004	**Mark Tuckerman**, Department of Chemistry and Courant Institute, New York University *A dual length scale approach to mixed quantum mechanical/molecular mechanical (QM/MM) simulations*
Special date **Tu 06.** 07. 2004 11:15, NC 5/99	**Klaus Hermann**, Fritz-Haber Institut, Berlin *Electronic and vibrational excitations at oxide surfaces: cluster models for vanadium oxide* (Joint seminar with SFB 558 "Heterogeneous Catalysis")
Special date **Tu 13.** 07. 2004 11:15, NC 5/99	**Sibylle Gemming**, Theoretische Physik, Technische Universität Chemnitz *Density-functional investigation of systems with reduced dimensionality* (Joint seminar with SFB 558 "Heterogeneous Catalysis")
14. 07. 2004	**Nisanth Nair**, Theoretische Chemie, Universität Hannover *Molecular Dynamics simulations using MSINDO*
Special date **Fr 16.** 07. 2004 **Time: 15:15**	**Gerald Mathias**, Biomolekulare Optik, Ludwig-Maximilians-Universität München *Description of long-range electrostatics in complex solvents by MD simulations: Angular dependence and range of dipolar ordering in water*
21. 07. 2004	**Marcel Baer**, Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum *Investigation on folding of the oligopeptide GVG(VPGVG)* (Joint seminar with FOR 436 "Water at Interfaces")
Special date **Th 22.** 07. 2004	**Jens Antony**, Numerische Mathematik, Freie Universität Berlin *Non-adiabatic effect in the amide-I Population Dynamics of glycine-dipeptide*
28. 07. 2004	**Peter Bloechl**, Theoretische Physik, Technische Universität Clausthal *How does nature break the strongest bond: First principles simulations of the enzyme nitrogenase*

gez. Die Dozenten der Theoretischen Chemie

Visitors are welcome to the seminar.