Lehrstuhl für Theoretische Chemie

Ruhr-Universität Bochum

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Theoretical Chemistry Colloquia (SS 2003)

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

23. 04. 2003	**Michel Mons**, Laboratoire Francis Perrin, Saclay/Gif-sur-Yvette Cedex, France *Laser spectroscopy of isolated biomolecules*
30. 04. 2003	no colloquium : Woche der Chemie im Ruhrpark Bochum
07. 05. 2003	**Bernd Meyer**, Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum *Composition and structure of complex surfaces: Combining DFT and thermodynamics*
14. 05. 2003	**Martin Kaupp**, Institut für Anorganische Chemie, Universität Würzburg *Density functional calculations of electronic g-tensors: methods and applications*
21. 05. 2003	**Ralph Jaquet**, Theoretische Chemie, Universität Siegen H_3^+
28. 05. 2003	no colloquium
04. 06. 2003	**Thierry Deutsch**, Laboratoire de Simulation Atomistique (CEA), Grenoble *Combining ab initio calculations and Monte Carlo simulations: Applications to Si with point defects* (Joint seminar with SFB 558 "Heterogeneous Catalysis")
11. 06. 2003	**Huib Bakker**, Ultrafast Spectroscopy, AMOLF, Amsterdam *Solvation and hydrogen-bond dynamics of water* (Joint seminar with FOR 436 "Water at Interfaces")
18. 06. 2003	**Konstantinos Kotsis**, Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum *Structure and UV/VIS spectra of ZnO complexes*
Special date **Tu 24.** 06. 2003 11:15, NC 5/99	**Christian Elsässer**, Fraunhofer-Institut für Werkstoffmechanik, Freiburg *Pd and Mo films on SrTiO_3 (001) surfaces - analysis of interfacial structure and bonding* (Joint seminar with SFB 558 "Heterogeneous Catalysis")
25. 06. 2003	**Anja Metzelthin**, Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum *Ab initio MD of the ammonia dimer*
02. 07. 2003	**Jozef Noga**, Slovak Academy of Sciences, Institute of Inorganic Chemistry, Bratislava *Towards the spectroscopic accuracy in quantum chemistry of small systems via explicitly correlated wave functions. The potential hypersurface of H_2O - H_2.*
09. 07. 2003	**Udo Schmitt**, Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum *Quantum dynamics of proton transport through complex hydrogen-bonded networks* (Joint seminar with FOR 436 "Water at Interfaces")
Special date 16. 07. 2003 **Time: 9:15**	**Martin Jungen**, Institut für Physikalische Chemie, Universität Basel *What is a muon doing in atoms or molecules?*
23. 07. 2003	no colloquium : ICQC Bonn
30. 07. 2003	**Kurt Binder**, Institut für Physik, Universität Mainz *Computer simulation of molten and glassy silica and its mixtures with sodium oxide and aluminium oxide*

gez. Die Dozenten der Theoretischen Chemie

Visitors are welcome to the seminar.