Lehrstuhl für Theoretische Chemie

Ruhr-Universität Bochum

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Theoretical Chemistry Colloquia (SS 2008)

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

09. 04. 2008	**Dr. Florian Janetzko**, Institut für Physikalische und Theoretische Chemie, Universität Bonn *Simulation of extended systems using the cyclic cluster model* (Speaker Exchange Program Bonn / Bochum)
16. 04. 2008	**Prof. Dr. Stefan Grimme**, Organisch-Chemisches Institut (Abt. Theoretische Chemie),Westfälische Wilhelms-Universität *Non-local Electron Correlation Effects and Non-covalent Interactions in Large Molecules* (Joint seminar with FOR 618 "Aggregation")
23. 04. 2008	**Prof. Dr. Wenjian Liu**, Institute for Theoretical and Computational Chemistry, College of Chemistry and Molecular Engineering, Peking University *Relativistic Theory for NMR Parameters*
30. 04. 2008	**Prof. Dr. Reinhold Fink**, Institut für Physikalische Chemie, Universität Würzburg *Understanding organic solar cells: A challenge for Quantum Chemistry*
07. 05. 2008	**M.Sc. Nina Winter**, Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum *Equilibrium structures of the adenine thymine base pair in the ground and first excited state*
14. 05. 2008	no colloquium
Special date **Mo 19.** 05. 2008 14:15, NC 03/399	**Dr. Mark Pederson**, Center for Computational Materials Science, Naval Research Lab.-639, Washington DC *Theory of Molecules and Clusters and Nanoscale Devices* (Joint seminar with SFB 558 "Heterogeneous Catalysis")
21. 05. 2008	no colloquium
Special date **Tu 27.** 05. 2008 11:15, NC 5/99	**Prof. Dr. Axel Groß**, Institut für Theoretische Chemie, Universität Ulm *Reactions at surfaces from first principles: energetics, dynamics and kinetics* (Joint seminar with SFB 558 "Heterogeneous Catalysis")
04. 06. 2008	**M.Sc. Janos Kiss**, Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum *Theoretical investigation of the high-pressure methanol synthesis process*
11. 06. 2008	**Dr. Michael Thoss**, Lehrstuhl für Theoretische Chemie, Technische Universität München *Quantum dynamics of charge transfer processes in the condensed phase*
18. 06. 2008	**Dr. Andreas Glöß**, Lehrstuhl Theoretische Chemie,Institut für Physikalische Chemie, Universität Karlsruhe *Efficient implementation of the MP2-R12 method for applications to large molecules* (Joint seminar with FOR 618 "Aggregation")
25. 06. 2008	**Dr. Florian Weigend**, Institut für Nanotechnologie, Forschungszentrum Karlsruhe *Density functional treatments of metal- and semi-metal clusters* (Joint seminar with SFB 558 "Heterogeneous Catalysis")
02. 07. 2008	no colloquium
09. 07. 2008	**Dr. Jordi Ribas Arino**, Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum *Several aspects of mechanochemistry: from thiolates adsorbed on gold surfaces to electrocyclic reactions*
Special date **Tu 15.** 07. 2008 11:15, NC 5/99	**Prof. Dr. Martin Schütz**, Institut für Physikalische und Theoretische Chemie, Universität Regensburg *Local correlation methods for excited states* (Joint seminar with SFB 558 "Heterogeneous Catalysis")
13. 08. 2008	**Dr. Lukasz Walewski**, Interdisciplinary Centre for Mathematical and Computational Modelling, University of Warsaw *Molecular simulations of proton transfer reaction in porphycene*

gez. Die Dozenten der Theoretischen Chemie

Visitors are welcome to the seminar.