Lehrstuhl für Theoretische Chemie

Ruhr-Universität Bochum

www.theochem.ruhr-uni-bochum.de

Theoretical Chemistry Colloquia (SS 2007)

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

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04. 04. 2007	**Jun Yang**, Institut für Theoretische Chemie, Universität Köln *DFT simulations of metal triborates containing Bi and lanthanides and evaluations of optical tensors for large systems in wavefunction-based approaches*
11. 04. 2007	**Christian Tuma**, Institut für Chemie, Humboldt-Universität Berlin *A QM/QM hybrid method for MP2/plane-wave-DFT studies of extended systems* (Joint seminar with SFB 558 "Heterogeneous Catalysis")
18. 04. 2007	**David E. Manolopoulos**, Physical & Theoretical Chemistry Laboratory, University of Oxford *Beyond quantum transition state theory: chemical reaction rates from ring polymer molecular dynamics* (Joint seminar with SFB 558 "Heterogeneous Catalysis")
25. 04. 2007	**David Tew**, Lehrstuhl für Theoretische Chemie, Universität Karlsruhe *New developments in R12 methods*
02. 05. 2007	**Harald Nieber**, Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum *Nonadiabatic ab initio molecular dynamics: photochemistry of biomolecules*
09. 05. 2007	**Otto E. Rössler**, Institut für Physikalische und Theoretische Chemie, Universität Tübingen *Origin of life*
16. 05. 2007	**Dusanka Janezic**, National Institute of Chemistry, Ljubljana *Computing infrared spectra for complex molecular systems* (Joint seminar with FOR 618 "Aggregation")
23. 05. 2007	**Darragh O'Neill**, Institut für Physikalische und Theoretische Chemie, Universität Mainz *Third-order properties in coupled-cluster theory*
30. 05. 2007	**Gero Schmidt**, Lehrstuhl für Theoretische Physik, Universität Paderborn *Organic molecule adsorption on solid surfaces from density-functional calculations*
06. 06. 2007	**Mark Tuckerman**, Department of Chemistry and Courant Institute, New York University *Ab initio molecular dynamics in the complete basis set limit using DVR techniques*
Special date **Tu 12.** 06. 2007 11.15, NC 5/99	**Christian Ochsenfeld**, Institut für Physikalische und Theoretische Chemie, Universität Tübingen *Quantum chemistry for large molecules: linear-scaling methods for mean-field and correlated approaches* (Joint seminar with SFB 558 "Heterogeneous Catalysis")
20. 06. 2007	**Philippe Hünenberger**, Physikalische Chemie, ETH Hönggerberg Zürich *The determination of single-ion solvation free energies: an experimental and theoretical puzzle* (Joint seminar with FOR 436 "Water at Interfaces")
27. 06. 2007	**Sara Bonella**, Department of Physics, University of Rome "La Sapienza" *Mixed quantum-classical approaches to nonadiabatic MD* ***- cancelled -***
Special date **Tu 03.** 07. 2007 11.15, NC 5/99	**Marco Bernasconi**, Department of Materials Science, University of Milano Bicocca *Chemical reactions at surfaces by ab-initio metadynamics* (Joint seminar with SFB 558 "Heterogeneous Catalysis")
11. 07. 2007	**Alessandro Laio**, Statistical and Biological Physics, SISSA Trieste *Recent developments of metadynamics* (Joint seminar with FOR 618 "Aggregation")

gez. Die Dozenten der Theoretischen Chemie

Visitors are welcome to the seminar.