

Lehrstuhl für Theoretische Chemie

Ruhr-Universität Bochum

www.theochem.ruhr-uni-bochum.de

Theoretical Chemistry Colloquia (WS 2013/2014)

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

16. 10. 2013 Paul Johnson, Department of Chemistry, McMaster University, Canada
Wavefunction Ansätze for Strongly-Correlated Systems
- Special date Festkolloquium zum 80. Geburtstag von Werner Kutzelnigg,
Th 24. 10. 2013 *International Symposium: 40 Years of Concepts in Theoretical Chemistry from
14:00, H-NC 30 the Bochum Perspective*
Neese, Werner, Köhn, Pulay, Jeziorski, Gauss, Valeev
13. 11. 2013 Jan Rossmeisl, Department of Physics, Technical University of Denmark
Room: NB 6/99 *Trends in electrocatalysis at the atomic scale*
-CANCELLED-
(Joint seminar with EXC 1069 "RESOLV")
20. 11. 2013 Martin Brehm, Wilhelm-Ostwald-Institut für Physikalische und Theoretische
Chemie, Universität Leipzig
TRAVIS - A Free Trajectory Analyzer
(Speaker Exchange Program Bonn / Bochum)
27. 11. 2013 Gemma Solomon, Nano-Science Center and Department of Chemistry,
University of Copenhagen
Chemical control of charge transport in molecular junctions
04. 12. 2013 Martin Zacharias, Physik-Department T38, Technische Universität München
*Simulation of nucleic acid and peptide dynamics using advanced sampling
methods*
(Joint seminar with EXC 1069 "RESOLV")
08. 01. 2014 Sho Imoto, Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum
*Theoretical methodology for calculating nonlinear (2D) IR spectra from MD
simulations*
(Joint seminar with EXC 1069 "RESOLV")
15. 01. 2014 Michele Ceriotti, Merton College, University of Oxford, UK
*Nuclear quantum effects in (first principles) molecular dynamics by colored-noise
thermostats*
29. 01. 2014 Marialore Sulpizi, Institute of Physics, Johannes Gutenberg Universität Mainz
*Water interfaces: structure and vibrational spectroscopy from DFT-based MD
simulations*
(Joint seminar with EXC 1069 "RESOLV")
- Special date Welcome of Lars Schaefer, Professor for Molecular Simulation, and his group,
05. 02. 2014
Time: 16:00

gez. Die Dozenten der Theoretischen Chemie
