

Lehrstuhl für Theoretische Chemie

Ruhr-Universität Bochum

www.theochem.ruhr-uni-bochum.de

Theoretisch-Chemisches Kolloquium (WS 2014/2015)

Zeit: mittwochs 14:15, Ort: Seminarraum NC 03/399

- Sondertermin** **Sergei Manzhos**, National University of Singapore, Singapore
Mo 22. 09. 2014 *Ab initio modeling of anode materials for Li, Na, and Mg ion batteries: post-Li issues, role of different phases, and computational matters*
Zeit: 15:15
05. 11. 2014 **David J. Huggins**, Cavendish Laboratory, Cambridge University, United Kingdom
Modelling Hydration With Inhomogeneous Fluid Solvation Theory
(Gemeinsames Seminar mit EXC 1069 "RESOLV")
12. 11. 2014 **Robert Wodraszka**, Lehrstuhl für Theoretische Chemie, Universität Bielefeld, Germany
The quantum dynamics of protonated methane and the Pauli principle
19. 11. 2014 **Sara Bonella**, Physics Department and CNISM, University of Rome "La Sapienza", Italy
Quantum effects via (almost) classical trajectories (?)
(Gemeinsames Seminar mit EXC 1069 "RESOLV")
26. 11. 2014 **Djurre de Jong-Bruinink**, Institut für Physikalische Chemie, Westfälische Wilhelms-Universität Münster, Germany
Simulating Proteins with the Coarse Grain Martini Force Field
(Gemeinsames Seminar mit EXC 1069 "RESOLV")
03. 12. 2014 **Kersti Hermansson**, Department of Chemistry, Uppsala University, Sweden
How different can water molecules be? - Insights into ion-water interactions from theoretical calculations for solids, solutions and surfaces
(Gemeinsames Seminar mit EXC 1069 "RESOLV")
- Sondertermin** **Andreas Dreuw**, Interdisciplinary Center for Scientific Computation, University of Heidelberg, Germany
Do 04. 12. 2014 *A quantum chemical view on mechanochemistry*
17:15, HNC 30 (Gemeinsames GDCh Kolloquium)
17. 12. 2014 **Jan Gerit Brandenburg**, Mulliken Center for Theoretical Chemistry, Institute for Physical and Theoretical Chemistry, Universität Bonn, Germany
Low-Cost Quantum Chemical Methods for Non-Covalent Interactions
(Seminar austauschprogramm Bonn / Bochum)
14. 01. 2015 **Michael Probst**, Forschungszentrum Ionen- und Plasmaphysik/Angewandte Physik, Universität Innsbruck, Austria
Ethylene Glycol and Water: News and Olds from Molecular Dynamics Simulations
(Gemeinsames Seminar mit EXC 1069 "RESOLV")
28. 01. 2015 **Thomas Kühne**, Department of Chemistry, University of Paderborn, Germany
Quantum Mechanics in a Glass of Water
(Gemeinsames Seminar mit EXC 1069 "RESOLV")

gez. Die Dozenten der Theoretischen Chemie

Gäste sind herzlich willkommen !