

# Lehrstuhl für Theoretische Chemie

## Ruhr-Universität Bochum

www.theochem.ruhr-uni-bochum.de

### Theoretical Chemistry Colloquia (WS 2014/2015)

---

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

---

- Special date**    **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*  
**Time: 15:15**    *issues, role of different phases, and computational matters*
05. 11. 2014    **David J. Huggins**, Cavendish Laboratory, Cambridge University, United Kingdom  
*Modelling Hydration With Inhomogeneous Fluid Solvation Theory*  
(Joint seminar with 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 (?)*  
(Joint seminar with 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*  
(Joint seminar with 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*  
(Joint seminar with EXC 1069 "RESOLV")
- Special date**    **Andreas Dreuw**, Interdisciplinary Center for Scientific Computation, University of  
**Th 04. 12. 2014** Heidelberg, Germany  
17:15, HNC 30 *A quantum chemical view on mechanochemistry*  
(Joint GDCh seminar)
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*  
(Speaker Exchange Program 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*  
(Joint seminar with EXC 1069 "RESOLV")
28. 01. 2015    **Thomas Kühne**, Department of Chemistry, University of Paderborn, Germany  
*Quantum Mechanics in a Glass of Water*  
(Joint seminar with EXC 1069 "RESOLV")

gez. Die Dozenten der Theoretischen Chemie

---

Visitors are welcome to the seminar.