

# Lehrstuhl für Theoretische Chemie

## Ruhr-Universität Bochum

www.theochem.ruhr-uni-bochum.de

### Theoretical Chemistry Colloquia (SS 2013)

---

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

---

24. 04. 2013 **Benjamin Helmich & Daniel Friese**, Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum  
*Analytic Hessians and vibrational spectra calculations for RI-CC2 and RI-MP2 & A low scaling pair natural approach for excited states*
12. 06. 2013 **Angelos Michaelides**, Theoretical Chemistry, London Centre for Nanotechnology, Room: NB 2/99 London  
*Towards accurate and reliable simulations of ice, water at surfaces, and some other things...*  
(Joint seminar with EXC 1069 "RESOLV")
- Special date** **Alexander Sokolov**, Center for Computational Quantum Chemistry, The University of Georgia, USA  
**Tu 18. 06. 2013**  
*Recent Developments in Density Cumulant Functional Theory*
19. 06. 2013 **Tobias Morawietz**, Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum  
*Development of Efficient and Accurate Potentials for the Simulation of Water Based on Artificial Neural Networks*
26. 06. 2013 **Stephan Ehrlich**, Mulliken Centre for Theoretical Chemistry, Institut für Physikalische und Theoretische Chemie, Universität Bonn  
*Dispersion Coefficients in DFT-D3: Development and Applications*  
(Speaker Exchange Program Bonn / Bochum)
17. 07. 2013 **Miriam Wollenhaupt**, Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum  
*Mechanochemistry of Cyclopropane Ring-Opening Reactions*

gez. Die Dozenten der Theoretischen Chemie

---

**Visitors are welcome to the seminar.**