

# Lehrstuhl für Theoretische Chemie

## Ruhr-Universität Bochum

www.theochem.ruhr-uni-bochum.de

### Theoretical Chemistry Colloquia (SS 2012)

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

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04. 04. 2012 no colloquium
11. 04. 2012 **Peter Schwerdtfeger**, Centre for Theoretical Chemistry and Physics, Massey University, Auckland  
*Spheres, Fullerenes and Hyperfullerenes*
18. 04. 2012 no colloquium
25. 04. 2012 **Piero Ugliengo**, Dipartimento Chimica IFM, University of Torino, Italy  
*Computational Simulations of Prebiotic Processes*  
(Joint seminar with SFB 558 "Heterogeneous Catalysis")
02. 05. 2012 **Alexander Urban**, Interdisciplinary Center for Molecular Materials (ICMM) and Computer-Chemistry-Center (CCC) Friedrich-Alexander-Universität Erlangen-Nürnberg  
*Crystal-field tight-binding as approximate DFT*  
(Joint seminar with SFB 558 "Heterogeneous Catalysis")
09. 05. 2012 **Waldemar Hujo**, Organisch-Chemisches Institut, Westfälische Wilhelms-Universität Münster  
*Accurate description of Ionic liquids, weak hydrogen bonds and thermochemistry by dispersion-corrected density functional theory*
16. 05. 2012 to be announced
23. 05. 2012 **Evert Jan Meijer**, Computational Chemistry and Physics Group, Amsterdam Center for Multiscale Modeling (ACMM), University of Amsterdam, The Netherlands  
*Understanding Aqueous Chemistry by Molecular Simulation*  
(Joint seminar with FOR 618 "Aggregation")
30. 05. 2012 **Dimitri G. Liakos**, Max-Planck-Institut für Bioanorganische Chemie, Mülheim a.d. Ruhr  
*Improved Correlation Energy Extrapolation Schemes based on Local Pair Natural Orbital Methods*
06. 06. 2012 to be announced
13. 06. 2012 **Thomas la Cour Jansen**, Faculty of Mathematics and Natural Sciences, University of Groningen, The Netherlands  
*The theory and simulation of two-dimensional vibrational spectroscopy*  
(Joint seminar with FOR 618 "Aggregation")
20. 06. 2012 to be announced
27. 06. 2012 **Till Westermann**, Theoretische Chemie, Fakultät für Chemie, Universität Bielefeld  
*First principle non-linear quantum dynamics using a correlation-based von Neumann entropy*
04. 07. 2012 **Ralf Ludwig**, Institute of Chemistry, University of Rostock  
*Effects of temperature, pressure and additives on the structure and dynamics of water*  
(Joint seminar with Research Department "IFSC")
11. 07. 2012 to be announced

gez. Die Dozenten der Theoretischen Chemie

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Visitors are welcome to the seminar.