# Lehrstuhl für Theoretische Chemie

# Ruhr-Universität Bochum

www.theochem.ruhr-uni-bochum.de

## Theoretical Chemistry Colloquia (SS 2012)

---

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

---

| | |
|---|---|
| 04. 04. 2012 | no colloquium |
| 11. 04. 2012 | **Peter Schwerdtfeger**, Centre for Theoretical Chemistry and Physics, Massey University, Auckland<br>*Spheres, Fullerenes and Hyperfullerenes* |
| 18. 04. 2012 | no colloquium |
| 25. 04. 2012 | **Piero Ugliengo**, Dipartimento Chimica IFM, University of Torino, Italy<br>*Computational Simulations of Prebiotic Processes*<br>(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<br>*Crystal-field tight-binding as approximate DFT*<br>(Joint seminar with SFB 558 "Heterogeneous Catalysis") |
| 09. 05. 2012 | **Waldemar Hujo**, Organisch-Chemisches Institut, Westfälische Wilhelms-Universität Münster<br>*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<br>*Understanding Aqueous Chemistry by Molecular Simulation*<br>(Joint seminar with FOR 618 "Aggregation") |
| 30. 05. 2012 | **Dimitri G. Liakos**, Max-Planck-Institut für Bioanorganische Chemie, Mülheim a.d. Ruhr<br>*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<br>*The theory and simulation of two-dimensional vibrational spectroscopy*<br>(Joint seminar with FOR 618 "Aggregation") |
| 20. 06. 2012 | to be announced |
| 27. 06. 2012 | **Till Westermann**, Theoretische Chemie, Fakultät für Chemie, Universität Bielefeld<br>*First principle non-linear quantum dynamics using a correlation-based von Neumann entropy* |
| 04. 07. 2012<br>**Room: NC 5/99** | **Ralf Ludwig**, Institute of Chemistry, University of Rostock<br>*Effects of temperature, pressure and additives on the structure and dynamics of water*<br>(Joint seminar with Research Department "IFSC") |
| 11. 07. 2012 | to be announced |

gez. Die Dozenten der Theoretischen Chemie

---

**Visitors are welcome to the seminar.**