# Lehrstuhl für Theoretische Chemie

# Ruhr-Universität Bochum

www.theochem.ruhr-uni-bochum.de

## Theoretical Chemistry Colloquia (WS 2007/2008)

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

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| 17. 10. 2007 | no colloquium |
| 24. 10. 2007 | **Taras Petrenko**, Theoretische Chemie, Universität Bonn<br>*Analysis and prediction of absorption bandshapes, fluorescence bandshapes, resonance Raman intensities and excitation profiles using the time dependent theory of electronic spectroscopy*<br>(Speaker Exchange Program Bonn / Bochum) |
| 31. 10. 2007 | no colloquium |
| 07. 11. 2007 | **Christoph Dellago**, Computational Physics Group, Universität Wien<br>*Transition path sampling simulations of phase transitions*<br>(Joint seminar with FOR 618 "Aggregation") |
| 14. 11. 2007 | **Jochen Schirmer**, Theoretische Chemie, Universität Heidelberg<br>*Is time-dependent density functional theory (TDDFT) formally exact?* |
| **Special date**<br>**Tu 20.** 11. 2007<br>11.15, NC 5/99 | **Walter Langel**, Institut für Biochemie, Universität Greifswald<br>*Simulations of titanium dioxide surfaces in real world systems*<br>(Joint seminar with SFB 558 "Heterogeneous Catalysis") |
| 28. 11. 2007 | **Hermann Gies**, Institut für Geologie, Mineralogie und Geophysik, Ruhr-Universität Bochum<br>*Minerals and prebiotic chemistry* |
| 05. 12. 2007 | **Alexander Witt**, Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum<br>*Quantum simulations of protonated methane: structure, IR spectra, and microsolvation* |
| **Special date**<br>**Tu 11.** 12. 2007<br>11.15, NC 5/99 | **Jörg Behler**, Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum<br>*Neural Network Potentials for Chemical Reactions: From Dynamics at Surfaces to Phase Transitions in Solids*<br>(Joint seminar with SFB 558 "Heterogeneous Catalysis") |
| 12. 12. 2007 | **Wolfgang Hieringer**, Theoretische Chemie, Universität Erlangen-Nürnberg<br>*Aspects of response property calculations using density-functional methods* |
| **Special date**<br>19. 12. 2007<br>14.15, **NB 2/99** | **Ulrich Heiz**, Physikalische Chemie, Technische Universität München<br>*Size effects in cluster catalysis*<br>(Joint seminar with SFB 558 "Heterogeneous Catalysis") |
| 09. 01. 2008 | **Hans Kricheldorf**, Institut für Technische und Makromolekulare Chemie, Universität Hamburg<br>*Polypeptides from alpha-Amino Acid-N-Carboxyanhydrides* |
| **Special date**<br>**Tu 15.** 01. 2008<br>14.15, **NC 03/399** | **Mark Waller**, Max-Planck-Institut für Kohlenforschung, Mülheim an der Ruhr<br>*Simulating the $^{51}$V Solid-State MAS NMR spectra of VCPO: A QM/MM Success Story* |
| 16. 01. 2008 | **Christoph van Wüllen**, Theoretische Chemie, Technische Universität Kaiserslautern<br>*Quantum chemical investigations on metal-catalyzed Michael reactions* |
| **Special date**<br>**Tu 22.** 01. 2008<br>11.15, NC 5/99 | **Nuria Lopez**, ICIQ Institut Català d' Investigació Química, Barcelona<br>*Different aspects of gold catalysis*<br>(Joint seminar with SFB 558 "Heterogeneous Catalysis") |
| 30. 01. 2008 | **Thomas Adler**, Theoretische Chemie, Universität Stuttgart<br>*Local explicitly correlated F12 theories* |
| 06. 02. 2008 | **Volker Blum**, Fritz-Haber-Institut der MPG, Berlin<br>*DFT and beyond with local orbitals - FHI-aims, a new all-electron/full-potential code*<br>(Joint seminar with SFB 558 "Heterogeneous Catalysis") |
| 13. 02. 2008 | **Yoshitaka Tateyama**, National Institute for Materials Science, Tsukuba<br>*Photo- and Electro-chemical reactions by TDDFT propagation and CPMD energy gap schemes* |

gez. Die Dozenten der Theoretischen Chemie

**Visitors are welcome to the seminar.**