

# Lehrstuhl für Theoretische Chemie

## Ruhr-Universität Bochum

www.theochem.ruhr-uni-bochum.de

### Theoretisch-Chemisches Kolloquium (WS 2015/2016)

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Zeit: mittwochs 14:15, Ort: Seminarraum NC 03/399

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21. 10. 2015 **Nisanth Nair**, Department of Chemistry, Indian Institute of Technology Kanpur, India  
*Development of CPMD-GULP QM/(polarized-) MM Interface for Modeling Extended Solids and Interfaces*  
(Gemeinsames Seminar mit EXC 1069 "RESOLV")
11. 11. 2015 **Janos Daru**, Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum  
*Enhanced sampling techniques for rare event systems*
18. 11. 2015 **Massimo Delle Piane**, Department of Chemistry, University of Torino, Italy  
*Large Scale QM Simulations of Periodic Systems: The Cases of Mesoporous Silica and Protein Crystals*  
(Gemeinsames Seminar mit EXC 1069 "RESOLV")
25. 11. 2015 **Alexander Schneider**, Mulliken Center for Theoretical Chemistry, Institute for Physical and Theoretical Chemistry, Universität Bonn  
*Boron-bearing molecules enclathrated in sodalites: Comparison of theory and experiment*  
(Seminar austauschprogramm Bonn / Bochum)
02. 12. 2015 **Mariana Rossi Carvalho**, Department of Chemistry, University of Oxford, UK  
*Nuclear quantum effects in biologically relevant systems from first principles*  
(Gemeinsames Seminar mit EXC 1069 "RESOLV")
09. 12. 2015 **Ali Alavi**, Max Planck Institute for Solid State Research, Stuttgart  
*Quantum Monte Carlo approach to the Full CI problem*
16. 12. 2015 **RESOLV-Kolloquium**  
**Raum: ND 03/99** **Thomas Frauenheim**, Bremen Center for Computational Materials Science, Universität Bremen  
*Recent DFTB extension for improving accuracy and boosting the efficiency for computational applications to nanomaterials*  
(Gemeinsames Seminar mit EXC 1069 "RESOLV")
- Sondertermin** **RESOLV-Kolloquium**  
13. 01. 2016 **Daniel Seeliger**, Boehringer Ingelheim Pharma GmbH & Co. KG Lead  
**Raum: HNC 10** *Identification and Opt. Support, Ingelheim*  
*Computational Chemistry in the Drug Discovery Industry*  
(Gemeinsames Seminar mit EXC 1069 "RESOLV")
20. 01. 2016 **Dirk Andrae**, Theoretische Chemie, Freie Universität Berlin  
*Chemical Bonding and Electronic States*
27. 01. 2016 **Gunnar Schmitz**, Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum  
*On the efficient combination of PNOs with F12 Theory: More than the sum of its parts*
03. 02. 2016 **Niels Hansen**, Institut für Technische Thermodynamik und Thermische Verfahrenstechnik, Universität Stuttgart  
*Stability of proteins and supramolecular complexes studied by molecular dynamics free-energy simulations*  
(Gemeinsames Seminar mit EXC 1069 "RESOLV")

gez. Die Dozenten der Theoretischen Chemie

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**Gäste sind herzlich willkommen !**