Lehrstuhl für Theoretische Chemie

Ruhr-Universität Bochum

www.theochem.ruhr-uni-bochum.de

Theoretisch-Chemisches Kolloquium (SS 2015)

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

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08. 04. 2015 **Prashant Kumar Gupta**, Department of chemistry, University of Basel, Switzerland
Computational exploration of water structure and dynamics at heterogeneous interfaces
(Gemeinsames Seminar mit EXC 1069 "RESOLV")

15. 04. 2015 **Jeremy O. Richardson**, Interdisciplinary Center for Molecular Materials (ICMM), Institute for Theoretical Physics, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany
Simulating electron-transfer processes with nonadiabatic ring-polymer molecular dynamics

22. 04. 2015 **Sereina Riniker**, Laboratory for Physical Chemistry, ETH Zürich, Switzerland
On the principles of coarse-graining
(Gemeinsames Seminar mit EXC 1069 "RESOLV")

06. 05. 2015 **Igor Schapiro**, Centre national de la recherche scientifique (CNRS), Institut de Physique et Chimie des Materiaux de Strasbourg, Universite de Strasbourg, France
Understanding Isomerization - Insight from hybrid QM/MM molecular dynamics simulations
(Gemeinsames Seminar mit EXC 1069 "RESOLV")

20. 05. 2015 **Mario Orsi**, School of Engineering and Materials Science, Queen Mary University of London, UK
Molecular simulations at different resolutions: atomistic, coarse-grained, and mixed
(Gemeinsames Seminar mit EXC 1069 "RESOLV")

03. 06. 2015 **Federica Agostini**, Theory Department, Max Planck Institute for Microstructure Physics, Germany
Coupled electron-nuclear dynamics in non-adiabatic process: The exact factorization approach
(Gemeinsames Seminar mit EXC 1069 "RESOLV")

01. 07. 2015 **Nadine Schwierz**, Department of Chemistry, University of California Berkeley, USA
Fibril growth of Ab40-pepetides: Thermodynamic and kinetic aspects
(Gemeinsames Seminar mit EXC 1069 "RESOLV")

08. 07. 2015 **Matthias Rupp**, Department of Chemistry, University of Basel, Switzerland
Machine Learning for Quantum Chemistry

15. 07. 2015 **Michael von Domaros**, Mulliken Center for Theoretical Chemistry, Institute for Physical and Theoretical Chemistry, Universität Bonn , Germany
Water Dynamics at a Janus Interface and in Extreme Nanoconfinement
(Seminaraustauschprogramm Bonn / Bochum)

29. 07. 2015 **Matti Hellström**, Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, Germany
Modelling Cu/ZnO with DFT: influence of band gap and band-filling problems

gez. Die Dozenten der Theoretischen Chemie

Gäste sind herzlich willkommen !