

Lehrstuhl für Theoretische Chemie

Ruhr-Universität Bochum

www.theochem.ruhr-uni-bochum.de

Theoretical Chemistry Colloquia (SS 2015)

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

08. 04. 2015 **Prashant Kumar Gupta**, Department of chemistry, University of Basel, Switzerland
Computational exploration of water structure and dynamics at heterogeneous interfaces
(Joint seminar with 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
(Joint seminar with EXC 1069 "RESOLV")
06. 05. 2015 **Igor Schapiro**, Centre national de la recherche scientifique (CNRS), Institut de
Physique et Chimie des Matériaux de Strasbourg, Université de Strasbourg, France
*Understanding Isomerization - Insight from hybrid QM/MM molecular dynamics
simulations*
(Joint seminar with 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
(Joint seminar with 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*
(Joint seminar with EXC 1069 "RESOLV")
01. 07. 2015 **Nadine Schwierz**, Department of Chemistry, University of California Berkeley, USA
Fibril growth of Ab40-peptides: Thermodynamic and kinetic aspects
(Joint seminar with 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
(Speaker Exchange Program 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

Visitors are welcome to the seminar.