Lehrstuhl für Theoretische Chemie

Ruhr-Universität Bochum

www.theochem.ruhr-uni-bochum.de

Theoretical Chemistry Colloquia (WS 2015/2016)

Time: wednesdays 14:15, Location: 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* (Joint seminar with 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* (Joint seminar with 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* (Speaker Exchange Program 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* (Joint seminar with 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 **Room: ND 03/99**	**RESOLV-Colloquium** **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* (Joint seminar with EXC 1069 "RESOLV")
Special date 13. 01. 2016 **Room: HNC 10**	**RESOLV-Colloquium** **Daniel Seeliger**, Boehringer Ingelheim Pharma GmbH & Co. KG Lead Identification and Opt. Support, Ingelheim *Computational Chemistry in the Drug Discovery Industry* (Joint seminar with 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* (Joint seminar with EXC 1069 "RESOLV")

gez. Die Dozenten der Theoretischen Chemie

Visitors are welcome to the seminar.