RUHR-UNIVERSITÄT BOCHUM

Center for Theoretical Chemistry

RUB

Theoretical Chemistry Colloquia (WS 2018/2019)

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

17. 10. 2018	**Giovanni Li Manni**, Department of Electronic Structure Theory, Max-Planck-Institut für Festkörperforschung, Stuttgart, Deutschland *Spin State Engergetics of Transition Metal Compounds from Modern Multireference Methods*
24. 10. 2018	**Michele Ceotto**, Dipartimento di Chimica, Università degli Studi di Milano, Milan, Italy *Semiclassical Methods for Spectroscopic Calculations of High Dimensional Molecular System* (Joint seminar with EXC 1069 "RESOLV")
31. 10. 2018	**Lisa Warczinski**, AG Quantenchemie, Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, Deutschland *Chemical Reactions at Carbon Surfaces: Computational Study and Method Development*
07. 11. 2018	**Krisztian Palotas**, Department of Theoretical Physics, Budapest University of Technology and Economics, Budapest, Hungary *Scanning Tunneling Microscopy Simulations from First Principles* (Joint seminar with EXC 1069 "RESOLV")
14. 11. 2018	**Jean-Philip Piquemal**, Laboratoire de Chimie Théorique, Sorbonne Université, Paris, France *Tinker-HP, a Massively Parallel Package for Scalable Polarizable and Hybrid Molecular Dynamics*
21. 11. 2018	**Ralph Jaquet**, Theoretische Chemie, Universität Siegen, Deutschland *Investigation of Nonadiabatic Effects for the Ro-vibrational Spectrum of H3+ using Geometry-dependent Nuclear Masses*
28. 11. 2018	**Fabian Bohle**, Mulliken Center for Theoretical Chemistry, Rheinische Friedrich-Wilhelms-Universität Bonn, Deutschland *Computation of Molecular Recognition Processes in Solution* (Speaker Exchange Program Bonn/Bochum)
05. 12. 2018	**Martin Zacharias**, Physik-Department, Technische Universität München, Deutschland *Investigating DNA Recognition and Repair Using Advanced Sampling Simulations* (Joint seminar with EXC 1069 "RESOLV")
12. 12. 2018	**Oriol Vendrell**, Lehrstuhl für Theoretische Chemie, Physikalisch-Chemisches Institut, Universität Heidelberg, Deutschland *Correlated Dynamics of Nuclei, Electrons and Trapped Photons*
Cancelled 09. 01. 2019	**Reinhard Dörner**, Institut für Kernphysik, Goethe-Universität, Frankfurt am Main, Deutschland *Imaging of Molecular and Electronic Structure*

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16. 01. 2019	**Dieter Gerlich**, Institut für Physik, Technische Universität Chemnitz, Deutschland *IR Spectroscopy of Cold Trapped Molecular Ions Using He-tagging* (Joint seminar with EXC 2033 "RESOLV")
23. 01. 2019	**Christoph Dellago**, Fakultät für Physik, Universität Wien, Österreich *Exploring the Mechanism and Kinetics of Nucleation Processes: From Ice Nucleation to Cavitation in Water under Tension* (Joint seminar with EXC 2033 "RESOLV")
30. 01. 2019	**Jérôme Hénin**, Laboratoire de Biochimie Théorique, Institut de Biologie Physico-Chimique, CNRS, Paris, France *Adaptive Sampling Based on Collective Variables in Biomolecular Simulations* (Joint seminar with EXC 2033 "RESOLV")
Special date 06.02.2019	**Özlem Yönder**, AG Quantenchemie, Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, Deutschland *Atomistic Multiscale Simulation of Char Combustion*

gez. Die Dozenten der Theoretischen Chemie

Guests are most welcome!