

Theoretical Chemistry Colloquia (SS 2019)

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

17. 04. 2019 **Reinhard Dörner**, Institut für Kernphysik, Goethe-Universität, Frankfurt am Main, Deutschland
Imaging of Molecular and Electronic Structure
- Special date**
Thu 02. 05. 2019 **Henrik R. Larsson**, Chemistry and Chemical Engineering, California Institute of Technology, California, USA
Applying Tensor Decompositions to Vibrational and Electronic Quantum Systems
15. 05. 2019 **Thomas Stockner**, Institute of Pharmacology, Center for Physiology and Pharmacology, Universität Wien, Österreich
How does ABCB1 harvest the energy of ATP for substrate transport?
(Joint seminar with EXC 2033 “RESOLV”)
22. 05. 2019 **Vahideh Alizadeh**, Institut für Physikalische und Theoretische Chemie, Mulliken Center for Theoretical Chemistry, Universität Bonn, Deutschland
Role of molecular modeling in the study of deep eutectic solvents
(Speaker Exchange Program Bonn/Bochum)
29. 05. 2019 **Attila Császár**, Laboratory of Molecular Structure and Dynamics, Institute of Chemistry, Eötvös University, Budapest, Hungary
Quasistructural Molecules
(Joint seminar with EXC 2033 “RESOLV”)
05. 06. 2019 **Florent Calvo**, Laboratoire Interdisciplinaire de Physique, Université Joseph Fourier Grenoble, France
Accounting for Quantum Nuclear Effects by Semiclassical Techniques Borrowed from the Energy Landscape Framework
(Joint seminar with EXC 2033 “RESOLV”)
- ZEMOS 0.17**
19. 06. 2019 **Gábor Csányi**, Department of Engineering, University of Cambridge, United Kingdom
A New Dawn for Interatomic Potentials
(Joint seminar with EXC 2033 “RESOLV”)
26. 06. 2019 **Mariusz Radón**, Department of Inorganic Chemistry, Faculty of Chemistry, Jagiellonian University, Krakow, Poland
Toward accurate spin-state energetics of transition metal complexes: benchmarking theory with respect to quantitative, environment-corrected experimental data
(Joint seminar with EXC 2033 “RESOLV”)
03. 07. 2019 **Benjamin Fingerhut**, Max-Born-Institut (MBI), Berlin, Deutschland
Noncovalent Interactions of Hydrated DNA and RNA Mapped by 2D-IR Spectroscopy
(Joint seminar with EXC 2033 “RESOLV”)

10.07.2019

Alexandre Tkatchenko, RU Physics and Materials Science, Université du Luxembourg, Luxembourg

Towards Universal Machine Learning Model of Molecular Properties in Chemical Space

(Joint seminar with EXC 2033 “RESOLV”)

gez. Die Dozenten der Theoretischen Chemie

Guests are most welcome!