RUHR-UNIVERSITÄT BOCHUM

Center for Theoretical Chemistry

RUB

Theoretical Chemistry Colloquia (SS 2022)

Time: Wednesdays 14:15, Location: Seminarraum NC 5/99

All Theoretical Chemistry Colloquia will be announced on an individual basis.,

27. 04. 2022 **Archy Tripathi**, Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, Deutschland
Deposition of a pure solid hydrogen matrix using Path Integral simulations

04. 05. 2022 **Dr. Chanbum Park**, Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, Deutschland
Deciphering Hydrogen Bonding at the Gold/Water Interface down to the Electronic Structure Level

11. 05. 2022 **Professor Ralf Drautz**, Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), Ruhr-Universität Bochum, Deutschland
Atomic Cluster Expansion for fast and accurate Interatomic Potentials
(Joint seminar with EXC 2033 "RESOLV")

18. 05. 2022 **Dr. Saumyak Mukherjee**, Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, Deutschland
Water entropy calculations in high-concentration protein solutions

01. 06. 2022 **Dr. Jan-Michael Mewes**, Mulliken Center for Theoretical Chemistry, Rheinische Friedrich-Wilhelms-Universität Bonn, Deutschland
What do signet-triplet gaps of charge-transfer states, periodic trends in melting and boiling points, and London-dispersion effects have in common?

15. 06. 2022 **Dr. Michael Häfner**, Mulliken Center for Theoretical Chemistry, Rheinische Friedrich-Wilhelms-Universität Bonn, Deutschland
Exploring the Chemistry of the Alkali Halide F Center
(Speaker Exchange Program Bonn/Bochum)

22. 06. 2022 **apl. Prof. Dr. Karin Fink**, Karlsruhe Institut of Technology, Institute for Nanotechnology, Karlsruhe, Deutschland
Quantum chemistry from molecules to materials

29. 06. 2022 **Juniorprofessor Jan Meisner**, Institut für Physikalische Chemie, Mathematisch-Naturwissenschaftliche Fakultät, Heinrich-Heine Unversität Düsseldorf, Deutschland
Reaction Discovery by Accelerated Molecular Dynamics
(Joint seminar with EXC 2033 "RESOLV")

06. 07. 2022 **Professor Kai Leonhard**, Lehrstuhl für Technische Thermodynamik, RWTH Aachen, Deutschland
Exploring Reaction Network with ChemTraYzer

14. 09. 2022 **Dr. Christoph Schran**, Department of Chemistry, University of Cambridge, United Kingdom

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Understanding complex aqueous systems with machine learning
(Joint seminar with EXC 2033 “RESOLV”)

gez. Die Dozenten der Theoretischen Chemie

Guests are most welcome!