

Sunday, 10.03.2019

18:00 Dinner
 19:15 – 20:00 Review and Perspectives: What's next?
 Ralf Ludwig

Monday, 11.03.2019

Catalysis & Metal Clusters

08:30 – 08:55 Synthesis of Manganese Complexes for the CO₂ Reduction.
 David Kotwica
 09:05 – 09:30 Investigations of Earth Abundant Metal based Catalysts for CO₂ Reduction.
 Elisabeth Oberem
 09:40 – 10:05 Neutral Clusters with Bromides as Inner Sphere Ligands.
 Loai Al Sheakh

10:15 Coffee break

NMR

10:45 – 11:10 Fast Field Cycling NMR Relaxometry – Limits and Future Perspectives.
 Anne Strate
 11:20 – 11:45 Dynamic Investigations of Ionic Liquids by NMR Relaxometry.
 Viviane Overbeck

12:30 Lunch

NMR & MD

15:00 – 15:25 Computing NMR Properties of Liquid Methanol from a Combination of Molecular Dynamics Simulation and *Ab Initio* Calculations.
 Chair: B. Golub
 Johanna Busch

15:35 – 16:00 Hydrogen Bond Dynamics in Ionic Liquids.
 Jan Neumann

16:15 Coffee break
 16:30 Gathering and discussion of current work in plenum.
 18:00 Dinner

Tuesday, 12.03.2019

Infrared Spectroscopy

08:30 – 08:55 Determination of the Strength of Intramolecular Hydrogen Bonding with Thermodynamic Methods and Infrared Spectroscopy.
 Riko Stewart
 09:05 – 09:30 Hydrogen Bonds and Dispersion Forces in Trialkylammonium-based Ionic Liquids.
 Peter Stange
 09:40 – 10:05 Chain Length Dependence of the Formation of Cationic Clusters: Influence on the Cation and Anion Dependence.
 Thomas Niemann

10:15 Coffee break

Molecular Dynamics Simulations

10:45 – 11:10 On the Balance Between Contact and Solvent-Separated Ion-Pairs in Mixtures of the Protic Ionic Liquid Triethylammonium-Methylsulfonate with Water.
 Dietmar Paschek
 11:20 – 11:45 Polarizable Simulations using CHARMM.
 Benjamin Golub

12:30 Lunch

Quantum Cluster Equilibrium (QCE)

15:00 – 15:25 The Quantum Cluster Equilibrium (QCE) Theory – Basics and Frank Weinholds Implementation.
 Andreas Appelhagen
 15:35 – 16:00 The Quantum Cluster Equilibrium (QCE) Theory – modern Application and the Peacemaker software.
 Sebastian Fritsch

16:15 Coffee break
 16:45 Gathering and discussion of current work in plenum.
 18:00 Dinner

Wednesday, 13.03.2019

Various Topics

08:30 – 08:55 Nationale Forschungsdateninfrastruktur (NFDI).
 Ralf Ludwig
 09:05 – 09:30 Chemie-Studium in Uppsala: Erste Eindrücke.
 T. Radost Herboth
 09:40 – 10:05 Was haben Lederstrumpf, Hitler und JFK mit unserer Sprechweise zu tun? – Überlegungen zur Wissenschaftsrhetorik in Europa und den USA.
 Kira Ludwig

10:15 Coffee break

10:45 Time for work group affairs (Homepage, seminar...)

12:00 Loading up the cars!!!

12:30 Lunch

15:00 Visit of INNO HEAT GmbH in Schwerin