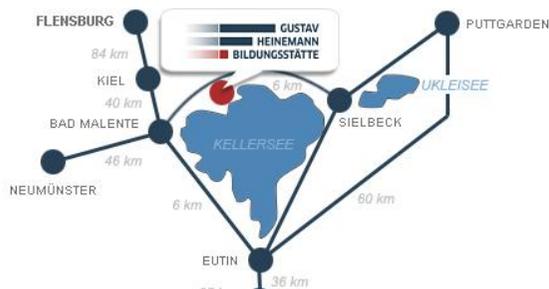


## Perspectives of Physical and Theoretical Chemistry



In this workshop we want to discuss our current status of our scientific work in a pleasant atmosphere. Out of the critical appraisal of the results and the introduction of new methodical approaches we want to evolve new perspectives for future projects.

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## Malente IX

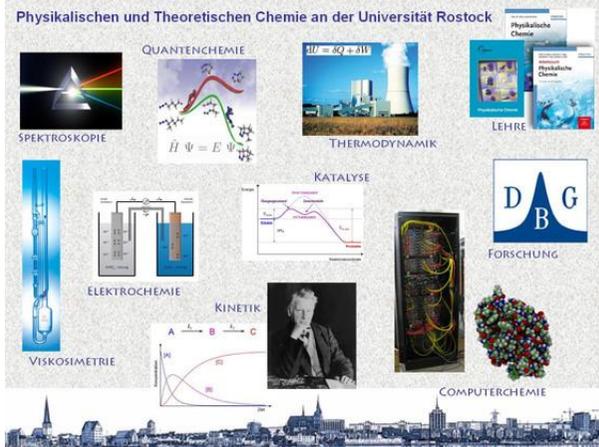


Image by Dr. J. Riemenschneider

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## Sunday, 07.02.16

18:00 Dinner

19:15 – 20:00 PTC: Review 2015 and Perspective 2016+.

Ralf Ludwig

## Monday, 08.02.16

MD & Spectroscopy

09:00 – 09:15 Development of an Infrared-spectroelectrochemistry cell.

Arend Rösel

09:25 – 09:40 Quantification of dispersion interactions in protic ionic liquids via far infrared spectroscopy.

Peter Stange

09:50 – 10:05 Structure and Dynamics in Mixtures of Protic Ionic Liquids: A Molecular Dynamics Simulation Study.

Benjamin Golub

10:15 Coffee break

10:45 – 11:00 Clusters of like-charged ions in ionic liquids.

Anne Knorr

11:10 – 11:25 Synthesis and characterization of OH-functionalized ionic liquids.

Thomas Niemann

11:35 – 11:50 A molecular dynamics simulation study of cation-cation interactions in cholinium based ionic liquids.

Jan Neumann

12:30 Lunch

15:00 – 15:15 N-methyl-6-hydroxyquinolinium bis(trifluoromethylsulfonyl)imide – Synthesis and Spectroscopy I.

Andranik Petrosyan

15:25 – 15:40 N-methyl-6-hydroxyquinolinium bis(trifluoromethylsulfonyl)imide – Synthesis and Spectroscopy II.

Stella Schmode

15:50 – 16:05 Dynamics of Ionic Liquids – From the Ultrafast to the Ultraslow: OHD-RIKES and FRAP Measurements.

Edward Quitevis

16:15 small break

16:30 Gathering and discussion of current work in groups

18:00 Dinner

## Tuesday, 09.02.16

NMR

09:00 – 09:15 Electrical Energy Storage by a Magnesium-Copper-Sulfide Rechargeable Battery.

Anne-Marie Bensa

09:25 – 09:40 NMR relaxation – Some principles and applications.

Alexander Wulf

09:50 – 10:05 Fast Field Cycling-NMR relaxometry: Basic principles and applications to solutions of LiNTf<sub>2</sub> in triglyme.

Andreas Appelhagen

10:15 Coffee break

10:45 – 11:00 Computing intermolecular magnetic dipolar relaxation rates from MD simulation: Possible pitfalls.

Dietmar Paschek

11:10 – 11:25 Deuteron Quadrupole Coupling Constants and Reorientational Correlation Times in Protic Ionic Liquids.

Matthias Strauch

11:35 – 11:50 Quadrupolar relaxation in mixtures of N-Methylacetamide and Ionic Liquids.

Viviane Overbeck

12:30 Lunch

MD & Theory

15:00 – 15:15 Temperature Dependence of the Osmotic 2<sup>nd</sup> Virial Coefficient of Apolar Particles in Aqueous Solutions.

Elias Reiter

15:25 – 15:40 Solubility Convergence and Criticality in Ionic Liquids.

Majid Namayandeh Jorabchi

15:50 – 16:05 Limitations of DFT calculations, for determining of guest-guest interactions in clathrat hydrates.

Wigbert Polet

16:15 small break

16:30 Gathering and discussion of current work in groups

18:00 Dinner

## Wednesday, 10.02.16

Catalysis

09:15 – 09:30 CO<sub>2</sub> reduction in Ionic Liquids.

Elisabeth Oberem

09:40 – 09:55 Role of Phosphin Ligands in Photocatalytic Hydrogen Production with Iron Carbonyls as Water Reduction Catalysts.

Steffen Fischer

10:15 Coffee break

10:45 Gathering and discussion of new perspectives in working groups

11:45 Working group reports in plenum

Loading up the cars

12:30 Lunch

Hurry! Departure to Dechow

14:30 Visit of Gläserne Molkerei Dechow

