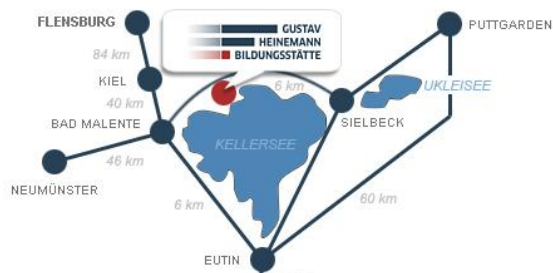


Perspectives of Physical and Theoretical Chemistry



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.

Gustav-Heinemann-Bildungsstätte (educational institution)
 Schweizer Straße 58
 D 23714 Bad Malente
 Fon + 49 (0)4523 – 88 09 70
 Fax + 49 (0)4523 – 88 09 728
 Mail info@heinemann-bildungsstaette.de



Malente XI

Physikalischen und Theoretischen Chemie an der Universität Rostock

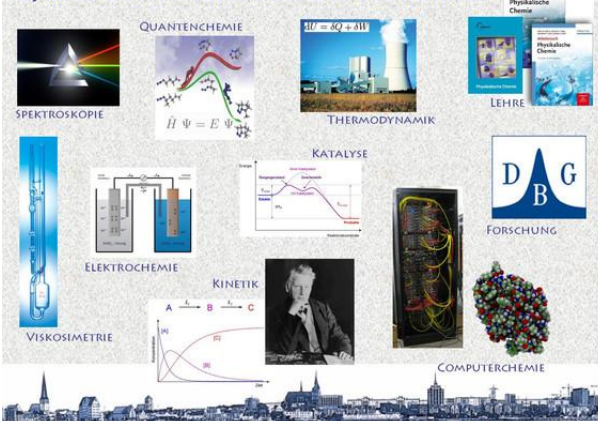


Image by Dr. J. Riemenschneider

organised by:

University of Rostock
 Physical and Theoretical Chemistry
 Prof. Dr. Ralf Ludwig
 Dr.-Lorenz-Weg 2
 D 18059 Rostock
 Fon + 49 (0)381 498-6517
 Fax + 49 (0)381 498-6524
ralf.ludwig@uni-rostock.de
www.ludwig.chemie.uni-rostock.de

Elisabeth Oberem
 Fon + 49 (0)381 498-8981
elisabeth.oberem@uni-rostock.de



Sunday, 18.03.2018

18:00 Dinner

19:15-20:00 Review and Perspectives: What's next?

Ralf Ludwig

Monday, 19.03.2018

Catalysis

08:30-08:55 Catalyst Poisoning due to Excess of Cocatalyst in Photocatalytic Water Reduction with Ironphosphides.

Steffen Fischer

09:05-09:30 Perspectives in the Manganese Catalyzed CO₂ Reduction

Elisabeth Oberem

09:40-10:05 DFT Calculations for Manganese Complexes.

David Kotwica

10:15 Coffee break

Quantum Chemistry

10:45-11:10 Hydrogen Gashydrates and Theoretical Calculated Ramanspectra.

Wigbert Polet

11:20-11:45 Salty Clathrates - Possibilities and Limitations

Sebastian Fritsch

12:30 Lunch

NMR

15:00-15:25 Is the Deuteron Quadrupole Coupling Constant Always a Constant?

Ralf Ludwig

15:35-16:00 H-bonds in Protic Ionic Liquids – Deuteron Quadrupole Coupling Constants and Dynamic Heterogeneities.

Peter Stange

16:15 Coffee break

16:30 Gathering and discussion of current work in plenum.

18:00 Dinner

Tuesday, 20.03.2018

NMR

08:30-08:55 Rotational Correlation Times, Diffusion Coefficients and Quadrupole Relaxation Enhancement in Protic Ionic Liquids by means of Field-Cycling NMR Relaxometry.

Viviane Overbeck

09:05-09:30 Analysis of Deuteron Relaxation Rates for Protic Ionic Liquids based on [(C_nH_{2n+1})₃ND]⁺ with n = 2; 6; 8.

Andreas Appelhagen

09:40-10:05 NMR Quadrupolar Relaxation in Water Revisited: Computing the ²H- and ¹⁷O-Relaxation in Liquid and Solid Water from Ab Initio Calculations and Molecular Simulations.

Dietmar Paschek

10:15 Coffee break

Ionic Liquids

10:45-11:10 Tuning Phosphonium Ionic Liquids with Ether Chains.

Frederik Philippi

11:20-11:45 Polarizable Simulations using GROMACS: First Results.

Benjamin Golub

12:30 Lunch

Ionic Liquids / Cationic Clusters

15:00-15:25 News and Perspectives from the Topic of Cationic Clusters.

Thomas Niemann

15:35-16:00 Hydrogen Bond Lifetimes in Ionic Liquids.

Jan Neumann

16:15 Coffee break

16:45 Gathering and discussion of current work in plenum.

18:00 Dinner

Wednesday, 21.03.2018

Various Topics

08:30- 08:55 Körpersprache - ein interaktiver Vortrag.

Kira Ludwig

09:05-09:35 Das Praktikum Physikalische Chemie - aktueller Stand und Perspektiven.

Alexander Wulf

09:45-10:00 Homepage Besprechung

10:15 Coffee break

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

12:00 Loading up the cars!!!

12:30 Lunch

14:00 Visit of GEOMAR Helmholtz-Zentrum in Kiel



Helmholtz-Zentrum für Ozeanforschung Kiel