

## GETTING HERE

How to get to Beckmanns Hof (IBZ) Universitätsstr. 150, 44801 Bochum: the best thing is to travel to the RUB and then go by foot. Walk past the university library and the Audimax, keep walking south and take the stairs right to the bottom (past the Mensa and Veranstaltungszentrum) until you reach the parking place near the Sport Halls. Leave the university campus and walk downhill, Beckmanns Hof is signposted from thereon.

RUHR-UNIVERSITÄT BOCHUM



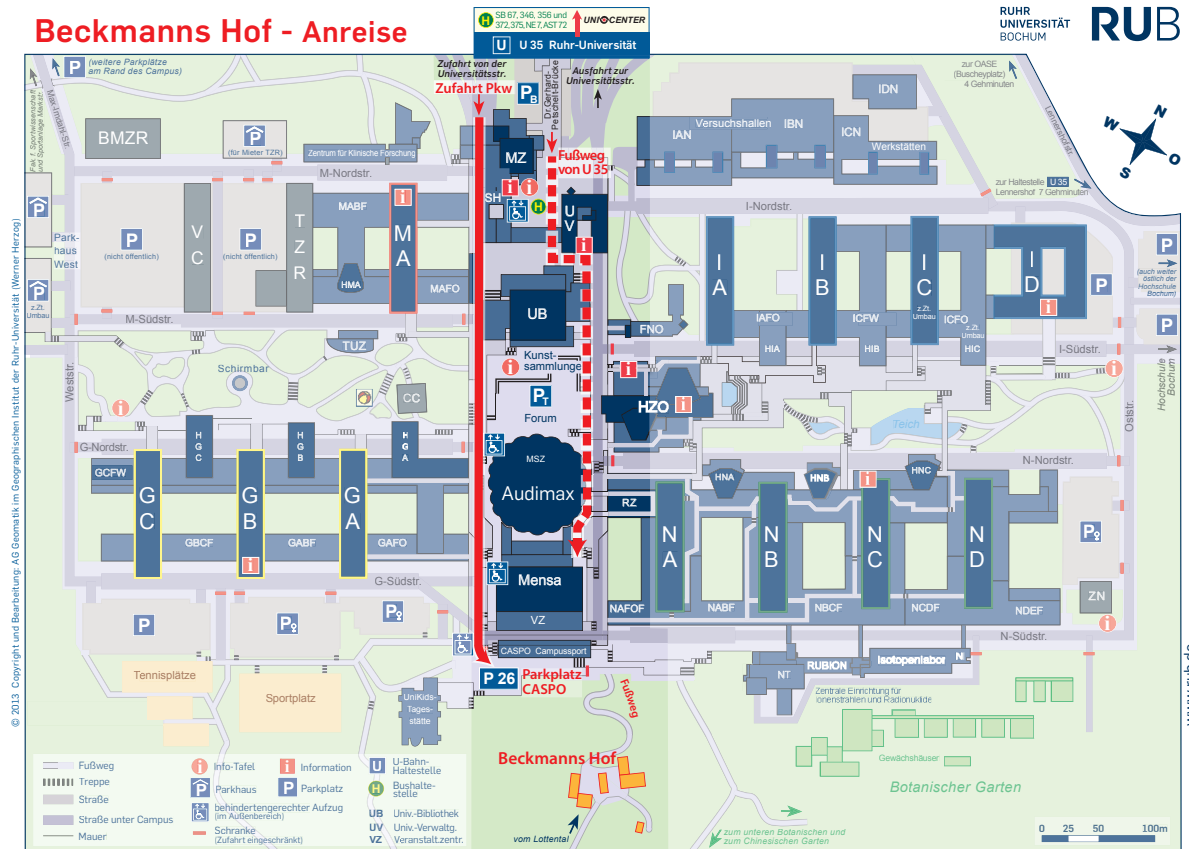
RUB

# GRADUATE SCHOOL SOLVATION SCIENCE (GSS) WORKSHOP

CLUSTER OF EXCELLENCE RESOLV

28<sup>th</sup> and 29<sup>th</sup> October 2013

RUHR-UNIVERSITÄT-BOCHUM  
BECKMANNS-HOF



RUHR-UNIVERSITÄT BOCHUM  
Cluster of Excellence RESOLV

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# PROGRAM

## 28.10.2013

Host: Simon Ebbinghaus

- 10:00 - 10:10 **Marcus Petermann**  
Dean of GSS welcomes all
- 10:10 - 10:40 **Martina Havenith-Newen**  
Coordinator of RESOLV  
„Solvation Science - New answers to an old problem“

Chair: Christian Müller

- 10:40 - 10:55 **Denise Heeskens**  
RUB Technical Chemistry  
„Liquid-phase oxidation of short-chain alcohols: Influence of the solvent and the catalyst support on activity and selectivity“
- 10:55 - 11:10 **Alexander Lüken**  
RUB Technical Chemistry  
„Liquid-phase alcohol oxidation investigated by ATR-IR spectroscopy and online mass spectrometry“

11:10 - 11:40 coffee break

- 11:40 - 11:55 **Kenny Bravo Rodriguez**  
MPI Kohlenforschung - Theoretical Chemistry  
„Computational studies of solvent effects in closed and open shell systems“

- 11:55 - 12:10 **Anna Katharina Kupka**  
RUB Anorganic Chemistry I  
„Influence on the crystallisation process of amino acids from solution“

- 12:10 - 12:25 **Demian Pitz**  
RUB Anorganic Chemistry III  
TBA

12:25 - 14:00 Lunch

Host: Andreas Erbe

- 14:00 - 15:00 **Christian Merten**  
RUB & MPI Kohlenforschung  
„How solvents influence conformations and configurations of chiral molecules“

Chair: Elsa Sanchez Garcia

- 15:00 - 15:15 **Elena Decaneto**  
MPI chem. Energiekonversion, Biosphys. Chem.  
„Cobalt Substitution in the Zinc Peptidase MMP14 for the Detailed Study of Its Enzymatic Activity and the Influence of Solvent“

- 15:15 - 15:30 **Tatiana Vasilevskaya**  
MPI Kohlenforschung, Theoretical Chemistry  
„QM/MM studies of matrix metalloproteinases“

- 15:30 - 15:45 **Tim Kothe**  
RUB Plant Biochemistry  
„Role of the solvent channel in the control of catalytic center solvation in Photosystem 2“

- 15:45 - 16:00 **Francesco Righetti**  
RUB Microbial Biology  
„The role of solvation in RNA structure dynamics“

- 16:00 - 16:15 **Fabian Klumpers**  
RUB Physical Chemistry I  
„Solvent's Impact on Protein Structure Formation, Conformational Stability and Intrinsically Disordered Proteins“

16:15 - 16:45 coffee break

Chair: Nathan Jukam

- 16:45 - 17:00 **Laura Wollny**  
RUB Physical Chemistry II  
„Developing a THz source for single-conformation spectroscopy of solute-solvent clusters“

- 17:00 - 17:15 **Christopher Norton**  
RUB Lehrstuhl für Thermodynamic  
„Concepts for a new magnetic suspension balance for the characterisation of two-dimensional surfaces“

- 17:15 - 17:30 **Matin Kaufmann**  
RUB Physical Chemistry II  
„Micro Solvation of Small Molecules in Helium Nanodroplets“

- 17:30 - 17:45 **Rainer Schulz**  
RUB Anorganic Chemistry II  
„Development of a real space DFT-method for the atomistic simulation of a charged liquid-solid interface“

17:45 - 20:30 Dinner & Poster Session

## 29.10.2013

Host: Tobias Fieback

- 09:00 - 10:00 **Matthias Heyden**  
MPI Kohlenforschung & RUB  
„Simulation and Solvation: atomistic insights into correlated solute-solvent dynamics“

Chair: Aliaksandr Bandarenka

- 10:00 - 10:15 **Martin Pogrzeba**  
MPI Eisenforschung Molecular Structures and Surface Design  
„Characterisation of electrochemical double layers after emersion at constant potential“

- 10:15 - 10:30 **Viktor Colic**  
RUB Analytical Chemistry  
„Tailoring the electrocatalytic activity with monolayer amounts of metals“

10:30 - 11:00 coffee break

- 11:00 - 11:15 **Alberto Ganassin**  
RUB Analytical Chemistry  
„A deeper insight into electrochemical gas evolution processes“

- 11:15 - 11:30 **Christoph Rösler**  
RUB Anorganic Chemistry II  
„Metal@ZIF: Catalyst for liquid phase aerobic alcohol oxidation“

- 11:30 - 11:45 **Tom Van Loo**  
Fraunhofer UMSICHT - RUB Technical Chemistry  
„Solid particle formation in and interaction with the liquid-phase - preparation and application of heterogeneous catalysts“

- 11:45 - 12:00 **Johannes Wiebe**  
Universität Duisburg-Essen, Theoretical Chemistry  
„Computer Simulation of Proton Discharge on Metal Electrodes“

- 12:00 - 12:15 **Mihaela Ivanova**  
RUB Lehrstuhl für Feststoffverfahrenstechnik  
„Supported Ionic liquid Phase (SILP) materials design in supercritical carbon dioxide and their applications in sorption processes“

- 12:15 - 12:30 **Jörg Behler**  
Coordinator ECR Board  
Closing Remarks