

INTERNATIONAL OPENING SYMPOSIUM OF THE CLUSTER OF EXCELLENCE RESOLV

4th and 5th June 2013

RUHR-UNIVERSITÄT-BOCHUM
VERANSTALTUNGSZENTRUM

GETTING HERE

■ By public transport

Bochum Central Station is served by ICE, IC, EC, regional, and suburban trains at a high frequency. From there, you can reach us easily by taking the underground line U35 (CampusLinie) straight to the Ruhr-Universität Bochum (RUB), which has its own station named after it. The U35 (direction Bochum Hustadt) runs at five-minute intervals on weekdays and takes just ten minutes to get to the university.

■ By car

Motorists can also easily reach the RUB via the dense network of motorways in Germany and especially in North Rhine-Westphalia. The quickest route is via the motorway junction Bochum/Witten, where the A43 and A44 meet. Simply take the exit Bochum-Querenburg, follow the signs "Ruhr-Universität" and then the (electronic) information boards.

■ By plane

Four airports – Dortmund, Münster/Osnabrück, Cologne/Bonn, and Düsseldorf – are within a reasonable distance of the RUB. Düsseldorf Airport, however, is not only the largest, but also the most easily accessed: there are direct connections between the airport and Bochum's main train station up to eight times per hour, and the journey only takes around half an hour.

REGISTRATION

Registration is free of charge.

Deadline for registration is Monday 20th May 2013. Please note that registration is only available online under

<http://www.ruhr-uni-bochum.de/solvation/opening>

and is **necessary** for participation.

There will be a Poster Session, if you are interested please use the above link to upload an abstract during registration.

Contact:

Coordinator: Prof. Dr. Martina Havenith-Newen

RUHR-UNIVERSITÄT BOCHUM

Exzellenzcluster RESOLV

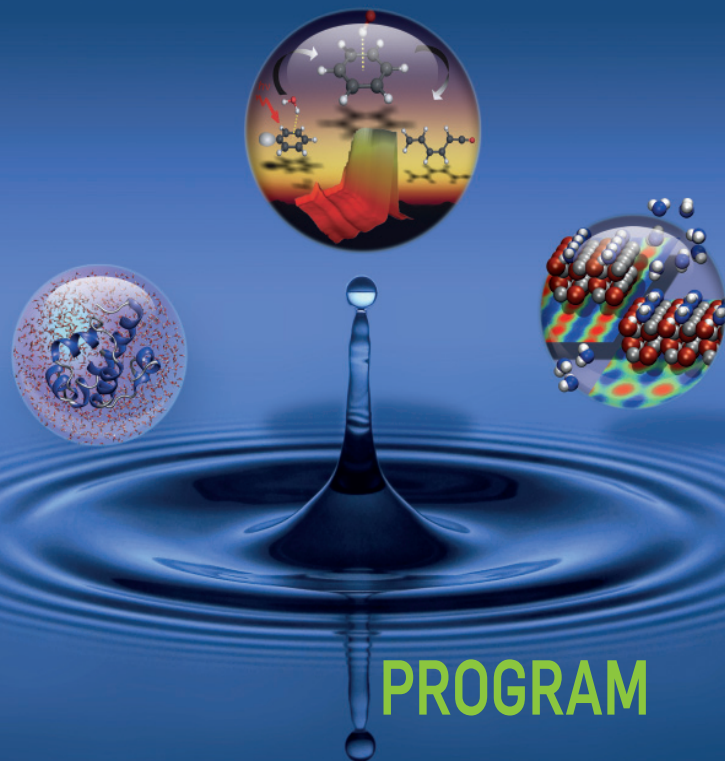
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PROGRAM

Program

June 3rd 2013

19:30 - 22:00 **Welcome Reception**

June 4th 2013

09:00 - 09:30 **Welcome**

- **Prof. Dr. E. Weiler**, Rector of the Ruhr University Bochum
- **Prof. Dr. M. Havenith**, Coordinator of RESOLV

09:30 - 09:40 **Musical Interlude**

09:40 - 10:20 **Philip Ball, Science Writer UK**
„From damnation to solvation“

10:20 - 10:50 *Coffee Break*

10:50 - 11:30 **Irit Sagi, Weizmann Institute, Israel**
„Site directed solvation dynamics mediates enzyme catalysis“

11:30 - 12:10 **Teresa Head-Gordon, UC Berkeley, USA**
„Dynamical environments and De Novo Enzymes“

12:10 - 12:50 **William L. Jorgensen, Yale University, USA**
„Drug Discovery Accelerated by Computational Methods“

12:50 - 14:20 *Lunch*

14:20 - 15:00 **Miguel A. Garcia-Garibay, UCLA, USA**
„Molecular rotors in amphidynamic crystals“

15:00 - 15:40 **Volkhard Helms, Saarland University, Germany**
„Structured solvent around biomolecules shapes the binding funnel“

15:40 - 16:20 **Daniel Borgis, École Normale Supérieure, France**
„Molecular Density Functional Theory approach to three-dimensional solvation“

16:20 - 16:50 *Coffee Break*

16:50 - 17:30 **Sabine Laschat, University of Stuttgart, Germany**
„Ionic liquid crystals - the charge makes the difference“

17:30 - 18:10 **David N. Reinhoudt, University of Twente, NL**
„From supramolecular chemistry to nanofabrication“

18:10 - 18:50 **Ursula Röthlisberger, EPFL, Switzerland**
TBA

June 5th 2013

09:00 - 09:40 **Angel E. Garcia, Rensselaer Polytechnic Institute, USA**
„Solvent and Co-solvent effects on biomolecular stability“

09:40 - 10:20 **Barry Carpenter, Cardiff University, UK**
„Energy Transfer: a Missing Factor in Common Solvation Models“

10:20 - 10:50 *Coffee Break*

10:50 - 11:30 **Ruth Gschwind, University of Regensburg, Germany**
„Solvent Effects in Organic, Bioorganic and Organometallic Chemistry Revealed by NMR“

11:30 - 12:10 **Peter Chen, ETH Zürich, Switzerland**
„Gas-phase organometallic thermochemistry: What do we learn about solution-phase chemistry?“

12:10 - 13:40 *Lunch*

13:40 - 14:20 **Huib J. Bakker, FOM, NL**
„Proton transfer and water dynamics at membrane surfaces“

14:20 - 15:00 **Timothy Zwier, Purdue University, USA**
„Solvent Effects on Vibronic Coupling in a Flexible Bichromophore: H₂O-mediated electronic localization and electronic energy transfer“

15:00 - 15:40 **Mark Johnson, Yale University, USA**
„Probing local solvent environments with isotopic labels using double resonance vibrational spectroscopy of cryogenic ions“

15:40 - 16:10 *Coffee Break*

16:10 - 16:50 **Hans Robert Kalbitzer, University of Regensburg, Germany**
„Detection of rare conformational states of proteins by high pressure NMR spectroscopy“

16:50 - 17:30 **Peter Hamm, University of Zürich, Switzerland**
„Towards a Molecular Understanding of Allosteric Dynamics by Ultrafast IR Spectroscopy“

17:30 - 18:10 **Martin Blackledge, Institut de Biologie Structurale J.P. Ebel, France**
„Functionally Important Conformational Dynamics in Folded and Intrinsically Unfolded Proteins from Nuclear Magnetic Resonance Spectroscopy“

18:10 - 18:30 **Closing Remarks**

18:30 - open end **Poster Session and BBQ**

