

Program GSS Summer School 2017

Tuesday, June 6

ZEMOS research building at the Ruhr-University Bochum

08:15 – 08:45 Registration
08:45 – 09:00 *Welcome*
 Matthias Heyden, MPI for coal research

Surface sensitive nonlinear spectroscopy

Chair: Patrick Nürnberger

09:00 – 10:30 Poul B. Petersen, Cornell University, USA
Introduction to surface nonlinear spectroscopy and applications to study water at interfaces and in biological settings

10:30 – 11:00 Coffee Break

11:00 – 12:00 Paul S. Cremer, Pennsylvania State University, USA
Probing Ion Binding and Water Structure at the Membrane Interface

12:00 – 13:00 John Conboy, University of Utah, USA
Sum-frequency vibrational spectroscopy for the study of lipid bilayer structure, compositional asymmetry and dynamics

13:00 – 14:30 Lunch

Molecular Simulations: Molecular Dynamic & Enhanced sampling

Chair: Christoph Schran

14:30 – 16:00 David van der Spoel, Uppsala University, Sweden
Computational Physical Chemistry of Liquids

16:00 – 16:30 Coffee Break

16:30 – 17:30 Ondrej Marsalek, Stanford University, USA
Properties of condensed-phase molecular systems from first principles

17:30 – 18:30 Mariana Rossi, Fritz Haber Institute, Berlin, Germany
Ab initio (quantum) molecular dynamics for H-bonded systems: Simulating (bio)molecules, condensed matter, and hybrid systems

19:15 Guided Tour through Bochum City

Wednesday, June 7

ZEMOS research building at the Ruhr-University Bochum

Molecular Simulations: Monte Carlo

Chair: Felix Uhl

- 08:30 – 10:00 Evert Jan Meijer, University of Amsterdam, The Netherlands
Principles of Monte Carlo Sampling
- 10:00 – 10:30 **Coffee Break**
- 10:30 – 11:30 David M. Ceperley, University of Illinois, USA
Understanding solvation in helium droplets with Path Integral Monte Carlo
- 11:30 – 12:30 Bettina Keller, FU Berlin, Germany
Analyzing Molecular Dynamics Simulations – Markov State Models and the Variational Approach to Molecular Dynamics
- 12:30 – 14:00 **Lunch**

Surface sensitive nonlinear spectroscopy

Chair: Matthias Heyden

- 14:00 – 15:30 Sylvie Roke, EPFL Lausanne, Switzerland
Nonlinear light scattering: molecular structure and electrostatic potentials on the nanoscale
- 15:30 – 16:00 **Coffee Break**
- 16:00 – 17:00 Hai-Lung Dai, Temple University, USA
Nonlinear Light Scattering from the surface of Colloidal Objects – from nanoparticles to biological cells
- 17:00 – 18:00 Yuki Nagata, Max Planck Institute for Polymer Research, Germany
Molecular Dynamics Simulation for Sum-Frequency Generation Spectra
- 18:00 – 18:30 **Career Day Introductory Workshop**

Thursday, June 8

ZEMOS research building at the Ruhr-University Bochum

Career Day

08:30 – 09:00 Reception with Coffee and Tea

09:00 – 09:10 Welcome
Dr. Matthias Heyden, MPI coal research

Chair: Akshay Raut

09:10 – 09:30 Dr. Christoph Weiß, CEO and founder, WSoptics, Altenstadt

09:30 – 09:50 Dr. Martin Bierbaum, European Patent Attorney

09:50 – 10:10 Dr. Marc Amkreutz, Computational Chemist, Fraunhofer IFAM, Bremen

10:10 – 10:30 Dr. Anja Metzelthin, Assistant to the Executive Board, German Physical Society, Bonn

10:30 – 11:00 Coffee Break

Chair: Reza Ghafarian Shirazi

11:00 – 11:20 Dr. Michael Bauer, CEO and founder, Carbolution Chemicals, St. Ingbert

11:20 – 11:40 Dr. Yvonne Neumann, Senior Technology Scout, Beiersdorf, Hamburg

11:40 – 12:00 Dr. Johannes Spenner, Quality Control Manager, Dynamit Nobel Explosiv- und Systemtechnik, Leverkusen

12:00 – 12:20 Dr. Christian Remenyi, Editor in Chief, Nachrichten aus der Chemie, Frankfurt

12:20 – 15:00 Career discussion with finger food/coffee (3 rounds á 45 min)

15:00 – 17:00 Panel discussion

17:00 Barbecue and Networking

Friday, June 9

RESOLV's participating institutes

Advanced Laboratory Modules