

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: TBA

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: TBA

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
TBA

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

Wednesday, June 7

ZEMOS research building at the Ruhr-University Bochum

Molecular Simulations: Monte Carlo

Chair: TBA

- 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
TBA
- 12:30 – 14:00 **Lunch**

Surface sensitive nonlinear spectroscopy

Chair: TBA

- 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 with guests from industry

09:00 – 12:30	Short Talks by Industry Guests
12:30 – 15:00	Lunch exchange with finger food
15:00 – 17:00	Panel discussion
17:00	Barbecue and Networking

Confirmed Speakers:

- Dr. Marc Amkreutz, Computational Chemist, Fraunhofer IFAM, Bremen
- Dr. Michael Bauer, CEO and founder, Carbolution Chemicals, St. Ingbert
- Dr. Martin Bierbaum, European Patent Attorney
- Dr. Yvonne Neumann, Senior Technology Scout, Beyersdorf, Hamburg
- Dr. Johannes Spenner, Head of Laboratory Analytics/Quality Control, Dynamit Nobel Explosiv- und Systemtechnik, Leverkusen
- Dr. Christoph Weiß, CEO and founder, Wsoptics, Altenstadt

Friday, June 9

RESOLV's participating institutes

Advanced Laboratory Modules