Berlin Center for Studies of Complex Chemical Systems

International Conference

Engineering of Chemical Complexity

4-8 July 2011, Harnack House,
Ihnestr. 16-20, Berlin (Dahlem)

Honorary Conference Chairman: G. Ertl

Organizing Committee: A. S. Mikhailov (chairman), M. Bär, E. Bodenschatz, H. Engel, M. Falcke, B. Fiedler, K. Krischer, J. Kurths, L. Schimansky-Geier, E. Schöll

Mini-Symposia and their Organizers: 1. *Wave Phenomena in Active Media* (H. Engel, M. Hauser, O. Steinbock), 2. *Reactive Gels* (I. Epstein), 3. *Chemical Oscillators* (I. Kiss and J. Kurths), 4. *Single Molecule Imaging and Manipulation* (L. Grill), 5. *Biochemical Evolution and Protocells* (K. Kaneko, S. C. Manrubia), 6. *Nonequilibrium Soft Matter* (M. Bär, T. Ohta), 7. *Electrochemistry and Surface Reactions* (J. L. Hudson, K. Krischer, H. H. Rotermund), 8. *Control of Self-Organization Processes* (E. Bodenschatz, E. Schöll), 9. *Active Particles* (L. Schimansky-Geier, K. Showalter), 10. *Applications to Cell Biology* (M. Falcke, S. Grill, T. Shibata), 11. *Stochastic Theory of Chemical Reactions* (K. Lindenberg, I. Sokolov), 12. *Networks* (S. Bornholdt, Th. Gross), 13. *Mathematical Aspects* (B. Fiedler, Y. Kevrekidis, Y. Nishiura)

Administrative assistance: P. Kaluza, I. Reinhardt, M Reimers, W. Mahdi, U. C. Künkel,
T. Reinhard, J. Löber, R. Buchholz

Supported by Deutsche Forschungsgemeinschaft (DFG), Solvay Company, SFB 910 “Control of Self-Organizing Nonlinear Systems”, Graduiertenkolleg 1558 “Nonequilibrium Collective Dynamics in Condensed Matter and Biological Systems”, and Fritz Haber Institute of the Max Planck Society

Program

Sunday, 3 July

16:00 – 20:00	Registration

Monday, 4 July

8:30 – 9:00	Registration
9:00 – 9:15	**G. Ertl**, Opening remarks
9:15 – 11:15	Symposium 1: **Wave Phenomena in Active Media**
11:15 – 11:45	Coffee break
11:45 – 12:45	Plenary lecture: **M. Eigen**
12:45 – 14:30	Lunch
14:30 – 16:30	Symposium 2: **Reactive Gels**
16:30 – 17:00	Coffee break
17:00 – 19:00	Symposium 3: **Chemical Oscillators**

Tuesday, 5 July

9:00 – 9:45	Plenary lecture: **T. Yanagida**
9:45 – 10:15	Coffee break
10:15 – 12:15	Symposium 4: **Single Molecule Imaging and Manipulation**
12:15 – 14:00	Lunch
14:00 – 16:00	Symposium 5: **Biochemical Evolution and Protocells**
16:00 – 16:30	Coffee break
16:30 – 18:30	Symposium 6: **Nonequilibrium Soft Matter**

Wednesday, 6 July

9:00 – 9:45	Plenary lecture: **P. Gaspard**
9:45 – 10:15	Coffee break
10:15 – 12:15	Symposium 7: **Electrochemistry and Surface Reactions**
12:15 – 14:00	Lunch
14:00 – 16:00	Symposium 8: **Control of Self-Organization Processes**
16:00 – 16:30	Coffee break
16:30 – 18:30	**Poster session I (Symposia 1 – 6)**
19:00 – 22:00	Conference dinner

Thursday, 7 July

9:00 – 9:45	Plenary lecture: **Q. Ouyang**
9:45 – 10:15	Coffee break
10:15 – 12:15	Symposium 9: **Active Particles**
12:15 – 14:00	Lunch
14:00 – 16:00	Symposium 10: **Applications to Cell Biology**
16:00 – 16:30	Coffee break
16:30 – 18:30	**Poster session II (Symposia 6 – 12)**

Friday, 8 July

9:00 – 9:45	Plenary lecture: **R. Kapral**
9:45 – 10:15	Coffee break
10:15 – 12:15	Symposium 11: **Stochastic Theory of Chemical Reactions**
12:15 – 14:00	Lunch
14:00 – 16:00	Symposium 12: **Networks**
16:00 – 16:30	Coffee break
16:30 – 18:30	Symposium 13: **Mathematical Aspects**

Plenary Lectures

1. **Manfred Eigen** (Max Planck Institute for Biophysical Chemistry, Göttingen, Germany)
Life: A manifestation of self-organized molecular complexity

2. **Toshio Yanagida** (Osaka University, Japan)
Single-molecule nanoscale imaging: Fluctuations and the function of life

3. **Pierre Gaspard** (Universite Libre de Bruxelles, Belgium)
Self-organization at the molecular level in far-from-equilibrium surface reactions and copolimerizations

4. **Qi Ouyang** (Peking University, Beijing, China)
Biological network reverse engineering in synthetic biology

5. **Raymond Kapral** (Toronto University, Canada)
Chemically-powered synthetic self-propelled nanomotors

Symposia

Symposium 1: **Wave Phenomena in Active Media**
Organized by H. Engel, M. Hauser, and O. Steinbock

1. **H. Engel**, Introduction (10 min)
2. **O. Steinbock**, Three-dimensional excitation waves (35 min)
3. **H. Stark**, Metachronal waves (25 min)
4. **K. Kruse**, Spontaneous protein waves in living cells (25 min)
5. **B. Echebarria**, Anomalous dispersion of pulse trains in excitable media with application to cardiac alternans (25 min)

Symposium 2: **Reactive Gels**
Organized by I. R. Epstein

1. **I. R. Epstein**, Introduction (10 min)
2. **R. Yoshida**, Self-oscillating polymer gels as smart materials (35 min)
3. **Y. Zhang, J. Delgado, N. Li, I. R. Epstein, B. Xu**, Responsive supramolecular hydrogels for chemomechanical systems (contributed, 25 min)
4. **J. Horváth, I. Szalai, P. De Kepper**, Rational experimental construction of chemomechanical oscillators with non-oscillatory reactions (contributed, 25 min)
5. **V. Yashin, O. Kuksenok, A. C. Balazc**, Computational design of active, self-reinforcing gels (contributed, 25 min)

Symposium 3: **Chemical Oscillators**
Organized by I. Z. Kiss and J. Kurths

1. **J. Kurths**, Introduction (5 min)
2. **A. F. Taylor**, Kinetic switches with catalytic particles coupled by chemical exchange (35 min)
3. **I. Z. Kiss**, Synchronization of small networks of electrochemical oscillators (20 min)
4. **A. Koseska, E. Volkov, J. Kurths**, Oscillation quenching mechanism: Amplitude *vs*. oscillation death (contributed, 20 min)
5. **C. Lenk, Ph. Maass, M. Köhler**, Synchronization of chemical oscillators undergoing the Belousov-Zhabotinsky reaction (contributed, 20 min)
6. **I. Lagzi, B. Kowalczyk, B. A. Grzybowski**, Chemical oscillations involving noble metal nanoparticles (contributed, 20 min)

Symposium 4: **Single Molecules Imaging and Manipulation**
Organized by L. Grill

1. **L. Grill**, Introduction (30 min)
2. **G. Meyer**, Scanning tunneling/atomic force microscopy of individual atoms/molecules on insulating films (35 min)
3. **T. Linderoth**, Molecular organization on surfaces studied by UHV-STM: Reaction, chirality and dynamics (35 min)
4. **S. Mülleger, M. Rashidi, R. Koch**, Spectroscopic signature of single Au(III) porphyrin cations on a gold surface (20 min)

Symposium 5: **Biochemical Evolution and Protocells**
Organized by K. Kaneko and S. C. Manrubia

1. **S. C. Manrubia**, Introduction (30 min)
2. **A. Libchaber**, Temperature gradient at the molecular scale: Soret effect, osmotic pressure and depletion force acting on RNA (40 min)
3. **K. Kaneko**, From catalytic networks to protocells (30 min)
4. **A. Kamimura, K. Kaneko**, Reproduction of a protocell by replication of minority molecule in a mutually catalyzing cycle (contributed, 20 min)

Symposium 6: **Nonequilibrium Soft Matter**
Organized by M. Bär and T. Ohta

1. **T. Ohta**, Introduction (10 min)
2. **T. Sugawara**, Self-reproduction of giant vesicles combined with amplification of encapsulated DNA (35 min)
3. **S. Alonso, M. Bär**, Modeling domain formation of high protein concentration at membranes of living cells (contributed, 20 min)
4. **H. Chaté**, Alignment *vs*. noise: Minimal models for collective motion (35 min)
5. **S. Thutupalli, R. Seemann, S. Herringhaus**, Hydrodynamic interactions in populations of simple model squirmers with tunable velocities (contributed, 20 min)

Symposium 7: **Electrochemistry and Surface Reactions**
Organized by J. L. Hudson, K. Krischer, and H. H. Rotermund

1. **K. Krischer**, Introduction (15 min)
2. **K. Sundmacher**, Dynamics of electrochemical CO oxidation in PEM fuel cells (45 min)
3. **K. A. Takeuchi, M. Sano**, Geometry-dependent universal fluctuations of growing interfaces: Evidence in turbulent liquid crystals (contributed, 20 min)
4. **A. Bernal-Osorio, M. Eiswirth**, Experimental observation of the effect of a low coupling strength on pattern formation during HCOOH electro-oxidation on a Pt ring electrode (contributed, 20 min)
5. **P. E. Klages**, *In-situ* visualization of pitting corrosion on stainless steel (contributed, 20 min)

Symposium 8: **Control of Self-Organization Processes**
Organized by E. Bodenschatz and E. Schöll

1. **E. Schöll**, Introduction (10 min)
2. **G. Seiden, S. Weiss, E. Bodenschatz**, Spatially forced thermal convection (30 min)
3. **S. Luther**, Timing electrical turbulence in the heart (30 min)
4. **M. A. Dahlem, E. Schöll**, Feedback control of 2D wave segments in cortical excitable media (30 min)
5. **S. Gurevich, R. Friedrich**, Destabilization of localized structures in reaction-diffusion systems induced by delayed feedback (contributed, 20 min)

Symposium 9: **Active Particles**
Organized by L. Schimansky-Geier and K. Showalter

1. **L. Schimansky-Geier**, Introduction
2. **A. Sen**, Collective dynamics of microswimmers (40 min)
3. **K. Showalter**, Motion analysis of self-propelled Pt-silica particles in hydrogen peroxide solutions (20 min)
4. **F. Sagués, P. Tierno**, Ratcheted colloids: From single particle enhanced diffusion to Rouse-like collective behavior (contributed, 20 min)
5. **P. Romanczuk, L. Schimansky-Geier**, Brownian particles with active fluctuations (contributed, 20 min)
6. **F. Peruani**, Transition to collective motion in bacterial colonies as a dynamical self-assembly of self-propelled rods (contributed, 20 min)

Symposium 10: **Applications to Cell Biology**
Organized by M. Falcke, S. Grill, and T. Shibata

1. **S. Sawai**, Spatial phase singularities and cell shape dynamics (45 min)
2. **T. Shibata**, Spontaneous symmetry breaking and signal processing in chemotactic response of eukaryotic cells (20 min)
3. **S. Grill**, Cellular polarization by coupling an active fluid to a pattern forming system (25 min)
4. **M. Enculescu, M. Falcke**, A model for the actin-based propulsion of spatially extended objects (contributed, 25 min)

Symposium 11: **Stochastic Theory of Chemical Reactions**
Organized by K. Lindenberg and I. Sokolov

1. **K. Lindenberg and I. Sokolov**, Introduction (15 min)
2. **D. T. Gillespie**, Stochastic chemical kinetics (45 min)
3. **V. Garcia-Morales, K. Krischer**, Enhancement of electrochemical reaction rates at the nanoscale, loss of correlations in electrochemical oscillators and superstatistics (contributed, 20 min)
4. **T. Kobayashi, A. Kamimura**, Reliable information processing in noisy intracellular networks (contributed, 20 min)
5. **Z. Hou**, Effects of internal noise in mesoscopic chemical oscillation systems: The stochastic normal form theory (contributed, 20 min)

Symposium 12: **Networks**
Organized by S. Bornholdt and Th. Gross

1. **Th. Gross**, Engineering self-organized criticality in adaptive networks (30 min)
2. **J. Davidsen, A. Shreim, A. Berdahi, F. Greil, M. Paczuski**, Attractor and basin entropies of random Boolean networks under asynchronous stochastic update (contributed, 20 min)
3. **M. Angeles Serrano, M. Boguna, F. Sagués**, Uncovering the hidden geometry behind methabolic networks (contributed, 20 min)
4. **H. Kori, Y. Kawamura, N. Masuda**, Network structure dependence of oscillation regularity in coupled noisy oscillators (contributed, 20 min)
5. **K. E. Bassler**, Co-evolutionary networks as a model for genetic regulation (30 min)

Symposium 13: **Mathematical Aspects**
Organized by B. Fiedler, Y. Kevrekidis, and Y. Nishiura

1. **Y. Nishiura**, Waves in heterogeneous media and their application to adaptive behavior of *Physarum plasmodium* (40 min)
2. **Y. Kevrekidis**, Coarse-graining dynamics on the networks, and of the networks (40 min)
3. **A. Mochizuki**, Identification of gene regulatory cycles: Applications (20 min)
4. **B. Fiedler**, Identification of gene regulatory cycles: Theory (20 min)

Abstracts

Plenary Lectures

(P1) Life: A Manifestation of Self-Organized Molecular Complexity

Manfred Eigen
Max Planck Institute for Biophysical Chemistry, Göttingen, Germany

(P2) Single Molecule Nano-Imaging: Fluctuations and the Function of Life

Toshio Yanagida
Graduate School of Frontier Bioscience Osaka University, Riken QBiC and NICT CiNet, 1-3, Yamadaoka, Suita, Osaka, 565-0871, Japan

Since biological molecular machines such as molecular motors, cell signal processors, DNA transcription processors and protein synthesizers are only nanometers in size and have a flexible structure, they are very prone to thermal agitation. Furthermore, the input energy level is not much different from that of average thermal energy, k_BT. Molecular machines can use this thermal noise with a high efficiency of energy conversion for their functions. This is in sharp contrast to man-made machines that operate at energies much higher than thermal noise. In recent years, single molecule imaging and nano-technologies have rapidly been expanding to include a wide range of life science applications. The dynamic properties of bio-molecules and the unique operations of molecular machines, which were previously hidden in averaged ensemble measurements, are now being unveiled. The aim of our research is to approach the engineering principle of adaptive biological systems by uncovering the unique operation of biological molecular machines. Here, I review our single molecule experiments designed to investigate molecular motors, enzyme reactions, protein dynamics and cell signaling, and discuss how thermal fluctuations (noise) play a positive role in the unique operation of biological molecular machines allowing for flexible and adaptive biological systems including cell and brain.

(P3) Self-Organization at the Molecular Level in Far-From-Equilibrium Surface Reactions and Copolimerizations

Pierre Gaspard
Department of Physics, Université Libre de Bruxelles, Belgium

Away from equilibrium, molecular processes acquire a directionality leading to self-organization down to the nanoscale, as a corollary of the second law of thermodynamics. This dynamical order arises in systems where spatial structuring is coupled to temporal ordering, as in the two nonequilibrium processes surveyed in this talk:

(I) With field ion microscopy, nanometric patterns are observed on multifaceted surfaces in the catalytic formation of water on rhodium [1,2,3]. These patterns find their origin in the anisotropy of the underlying crystal. Indeed, kinetic parameters such as the activation energies vary with the local Miller indices on the reacting surface. Other key features are the dependence of kinetic parameters on the local electric field, as well as the ultrafast surface diffusion of hydrogen atoms leading to their quasi-equilibrium spatial distribution [4].

Far from equilibrium, transitions happen to bistable and oscillating regimes. In these nonequilibrium regimes, the surface layer and sublayer have an organization different from the equilibrium structure.

(II) Nonequilibrium constraints also drive self-organization at the molecular level in copolymerizations with or without templates. As recently shown [5,6], the dissipation generated during these nonequilibrium processes turns out to be closely related to the information stored in the growing sequence of monomers, or transmitted between the template and the synthesized copolymer. At equilibrium, information transmission is no longer effective, which emphasizes the importance of nonequilibrium conditions to generate dynamical order, particularly, in biological systems.

[1] J.-S. McEwen, P. Gaspard, T. Visart de Bocarmé, and N. Kruse, Nanometric chemical clocks. Proc. Natl. Acad. Sci. USA, **106**, 3006 (2009).

[2] J.-S. McEwen, P. Gaspard, T. Visart de Bocarmé, and N. Kruse, Oscillations and Bistability in the Catalytic Formation of Water on Rhodium in High Electric Fields. *J. Phys. Chem. C,* **113**, 17045 (2009).

[3] J.-S. McEwen, P. Gaspard, T. Visart de Bocarmé, and N. Kruse, Electric field induced oscillations in the catalytic water production on rhodium: A theoretical analysis. *Surf. Sci.,* **604**, 1353 (2010).

[4] A. Garcia Cantu Ros, J.-S. McEwen, and P. Gaspard, Effect of ultrafast diffusion on adsorption, desorption, and reaction processes over heterogeneous surfaces. *Phys. Rev. E,* **83**, 021604 (2011).

[5] D. Andrieux and P. Gaspard, Nonequilibrium generation of information in copolymerization processes. *Proc. Natl. Acad. Sci. USA,* **105**, 9516 (2008).

[6] D. Andrieux and P. Gaspard, Molecular information processing in nonequilibrium copolymerizations. *J. Chem. Phys.,* 1**30**, 014901 (2009).

(P4) Biological Network Reverse Engineering in Synthetic Biology

Qi Ouyang

Center for Theoretical Biology and Department of Physics, Peking University, 100871, China

Synthetic biology is a new branch of interdisciplinary science that has been developed in recent years for the application of biological technology. The main purpose of synthetic biology is to develop basic biological functional modules, and through rational design, develop man-made biological systems that have predicted useful functions. In this talk, I will discuss two principles in rational design of functional biological circuits: the forward engineering design and the reverse engineering design. I will use a few synthetic biology researches that conducted in my laboratory at Peking University to illustrate the above principles: Synthesis of push-on-push-off biological switch; synthesis of “Bavulov bacteria”; and synthesis a cell which has a semi-log dose-response to the environment. These works demonstrate the potential application of network engineering in synthetic biology.

(P5) Chemically Powered Synthetic Self-Propelled Nanomotors

Raymond Kapral

Department of Chemistry, University of Toronto, Canada

Biological systems make frequent use of molecular motors to perform tasks such as active transport of material in the cell, cell locomotion and biochemical synthesis. Recently, chemists have fabricated a variety of synthetic nanomotors that use chemical reactions to effect self propulsion. Because of their potential applications, such synthetic nanodevices are being investigated actively. Like their biological counterparts, these nanomotors operate in the regime where they are subject to strong molecular fluctuations from the environments in which they move, and their motion is governed by viscous forces. The talk will describe recent experimental and theoretical work on various types of synthetic nanomotors, the means by which they move and some of their possible uses.

Symposium 1: **Wave Phenomena in Active Media**

(S01 – I) Introduction

H. Engel

Department of Physics, Technical University of Berlin, Germany

(S01 – T1) Three-dimensional excitation waves

Oliver Steinbock

Department of Chemistry and Biochemistry, Florida State University, Tallahassee, FL 32306-4390, USA

Much of this talk will focus on the pinning of scroll waves to unexcitable obstacles [1-3]. Scroll waves are the three-dimensional analogue of rotating spiral waves in two-dimensional active media but their rotation occurs around one-dimensional space curves called filaments. These filaments are dynamical objects and must obey strict topological constraints. In experiments with the Belousov-Zhabotinsky reaction and numerical simulations with excitable reaction-diffusion models, we study the anchoring and termination of filaments at inert obstacle of various shapes and sizes. In particular, I will present recent results on scroll wave pinning that involves a topological mismatch (e.g., a circular filament loop pinned to a double torus). The relevance of scroll wave pinning to cardiology will also be discussed.

[1] Z. Jiménez, B. Marts, O. Steinbock, *Phys. Rev. Lett.* **102**, 244101 (2009).
[2] Z. Jiménez, O. Steinbock, *Europhys. Lett.* **91**, 50002 (2010).
[3] S. Dutta, O. Steinbock, *J. Phys. Chem. Lett.* **2**, 945 (2011).

(S01 – T2) Metachronal waves in model systems

Holger Stark

Institute for Theoretical Physics, Technical University of Berlin, Germany

Microorganisms such as paramecium are covered by a carpet of beating filaments called cilia. The motion of these cilia is highly coordinated or synchronized so that so-called metachronal waves run along the cell surface. There is strong evidence that these waves are due to hydrodynamic interactions between the beating cilia, meaning that cilia interact with their neighbors via long-range flow fields they produce by their beating motion. In this talk I will present two model systems where we aim to develop an understanding under which conditions hydrodynamic interactions lead to metachronal waves. We first study a chain of driven oscillators also called rowers [1]. These are beads that move on straight line segments and that are driven by external forces. Our main observation is that metachronal waves occur only when we restrict the range of hydrodynamic interactions either artificially to nearest neighbors or by the presence of a bounding surface as in any relevant biological system. The second example presents a two-dimensional array of rods attached to a surface. We drive them by a torque along the surface of a cone tilted against the surface normal. For constant torque all the rods synchronize. However, if we divide the rod stroke in a fast transport and a slow recovery stroke, metachronal waves develop.

[1] C. Wollin and H. Stark. Metachronal waves in a chain of rowers with hydrodynamic interactions, *Eur. Phys. J. E* **34**, 42 (2011).

(S01 – T3) Spontaneous protein waves in living cells

Karsten Kruse
Department of Physics, University of the Saarland, Saarbrücken, Germany

(S01 – T4) Anomalous dispersion of pulse trains in excitable media with application to cardiac alternans

Blas Echebarria[1], G. Röder[2], H. Engel[3], J. Davidsen[4], and M. Bär[5]
[1] Dept. de Física Aplicada, Universitat Politècnica de Catalunya, Barcelona, Spain, [2] Max-Planck-Institut für Physik komplexer Systeme, Dresden, Germany, [3] Institut für Theoretische Physik, Technische Universität Berlin, Berlin, Germany, [4] Department of Physics and Astronomy, University of Calgary, Calgary, Canada, [5] Physikalisch-Technische Bundesanstalt, Berlin, Germany

Propagation of pulse trains in excitable media is usually characterized by a so-called dispersion curve that gives the velocity of a pulse in a periodic train as a function of its wavelength. Since a pulse typically is followed by a refractory zone of decreased excitability, the pulse velocity monotonically increases with increasing wavelength (= normal dispersion). In the context of excitable cardiac tissue, normal dispersion corresponds to normal conduction. Anomalous dispersion refers to an increase of pulse (or action potential) velocity with decreasing distance to the preceding pulse. We will show that the form of the dispersion curve has a very strong effect on the dynamics of cardiac alternans. This is a beat-to-beat alternation in the duration of the excited phase of the action potential (AP) that has been shown to be highly pro-arrhythmic. While normal dispersion promotes a heterogeneous distribution in the duration of the AP along tissue, known as discordant alternans, anomalous dispersion leads to AP pairs and bunching, and stabilizes concordant (i.e., in phase) alternans in arbitrarily long paced one-dimensional cables. As a consequence, spiral waves in two-dimensional tissue simulations exhibit straight nodal lines for anomalous dispersion in contrast to spiraling ones in the case of normal conduction.
[1] B. Echebarria, G. Röder, H. Engel, J. Davidsen, and M. Bär, *Phys. Rev. E,* **83**, R040902 (2011).

(S01 – P1) Self-organization and wave propagation in precipitate systems: Experiments and theoretical modeling

Mazen Al-Ghoul
Department of Chemistry and Center for Advanced Mathematical Sciences, American University of Beirut, P.O. Box 110236, Beirut, Lebanon

Pattern formation in precipitate systems is a fascinating self-organizing phenomenon that is encountered in numerous natural and chemical systems. It exhibits complex spatiotemporal dynamics such as static bands, propagating waves, and chaos. We present several precipitate systems that are currently under study in our laboratory, elucidate some aspects of their formation mechanism and introduce a theoretical model that describes them.

(S01 – P2) Dynamics of scroll waves in thin layers of the photosensitive Belousov-Zhabotinsky reaction

Arash Azhand, Rico Buchholz, Peter Kolski and Harald Engel
Institut für Theoretische Physik, TU Berlin, Hardenbergstraße 36, D-10623 Berlin

Undamped propagation of three-dimensional travelling waves has been observed in a variety of dissipative active media including chemical waves, temperature waves in solid fuel combustion and waves of electric activity during cardiac arrhythmias, for example. Here, we present experimental and numerical results for the evolution of scroll waves in thin layers of the photosensitive Belousov-Zhabotinsky reaction. The study is focused on boundary effects modifying the intrinsic wave dynamics in the unbounded medium. The analysis is performed in the excitable regime for parameter settings corresponding to both positive and negative filament tension. Experimental findings are compared to direct numerical simulations with the underlying Oregonator model. Our results do not depend, however, on a particular kinetics but apply to a large class of excitable media.

(S01 – P3) Studying pattern formation in reaction-diffusion-advection systems with microfluidic devices

Igal Berenstein, Robert Niedl, Carsten Beta
Biological Physics, Institute of Physics and Astronomy, University of Potsdam

We study pattern formation in reaction-diffusion-advection systems using microfluidic devices. Our approach is illustrated using the well-known Belousov-Zhabotinsky reaction, including a comparison of experimental results and numerical simulations. The advantages and drawbacks of microfluidic techniques for the study of nonlinear chemical systems are considered and future directions of research in this field are discussed.

(S01 – P4) Adsorption waves in reactive porous media used for solar energy storage

Domenico Bullara, Yannick De Decker
Nonlinear Physical Chemistry Unit, Service de Chimie Physique et Biologie Théorique, Faculté des Sciences,
Université Libre de Bruxelles (ULB), CP 231, Campus Plaine, 1050 Brussels, Belgium

A growing interest has recently developed on the possibility to exploit reversible exothermic chemisorption to efficiently store solar thermal energy for long, inter-seasonal periods of time. In particular, the chemisorption of water on inorganic salts proved to be especially suited to such applications. Thermogravimetric studies show a strong dependence of the rate of the global adsorption process with respect to the amount of salt, which is not coherent with a homogeneous chemical reaction. This effect could, in principle, be attributed to many different reasons, mainly related to anisotropies or heterogeneities in the solid matrix. We therefore built a model aimed at reproducing the most important trends of the experiments. We used the Dusty Gas Model coupled with Maxwell-Stefan relations for mass transfer, and a simple Langmuir kinetic for chemisorption. Numerical integrations showed the existence of a region of parameter space where traveling waves of adsorbed water can appear, as a consequence of the coupling between mass transport and chemical reaction. In this view, the occurrence of a wave-like phenomenon may explain the dependence of the global adsorption rate on the total amount of solid. Furthermore, the adsorption curves obtained in this regime closely reproduce the experimental ones, even in their finer details. These results show that coupling between mass transfer and adsorption is enough to explain the aforementioned intriguing experimental results, without the need to invoke spatial heterogeneities or more exotic effects.

(S01 – P5) A computer model to estimate the effects of cardiac motion on electrical excitation and the magnetocardiogram

Stefan Fruhner[1], Harald Engel[1], Markus Bär[2]

[1] Institut für Theoretische Physik, Technische Universität Berlin; [2] Physikalisch-Technische Bundesanstalt, Berlin

Computer models of cardiac excitation include a very precise physiological description and accurately account for anatomical details like fibre orientation or heterogeneity of heart tissue. On the other hand cardiac motion often is neglected whereas it might be essential for a deeper understanding of the mechanisms of cardiac arrhythmias like tachycardia and fibrillation. A tagged acquisition protocol for magnetic resonance images (MRI at DHZ Berlin) was chosen to extract cardiac motion for a set of tagged points within the myocardial region. Finite element meshes containing artificial allocated fibre directions were constructed for different temporal states of the human heart in order to perform simulations of waves of electrical activity. Intra- and extracellular domains are treated separately utilizing a bidomain approach. The experimentally estimated motion is included by implementing an interpolation method for transferring the ionic states and transmembrane voltages between different meshes. Comparisons are drawn to static simulations. To characterize these differences in simulations the activation times of the excitation have been computed. For the moving heart, in some regions activation times up to 20 ms smaller than in the static case have been obtained. At the same time other regions became activated 25 ms later. The impact of cardiac motion can also be demonstrated in artificially generated biosignals like the electrocardiogram (ECG) or the magnetocardiogram (MCG), where T-wave maximum occurs approximately 10–20ms earlier in the dynamic case.

(S01 – P6) Interaction of a pair of scroll waves

Dennis Kupitz, Marcus J. B. Hauser

Abteilung Biophysik, Institut für Experimentelle Physik, Otto-von-Guericke-Universität Magdeburg, Universitätsplatz 2, 39106 Magdeburg, Germany

Scroll waves are the three-dimensional counterparts of spiral waves occurring in excitable media. Single scroll waves may undergo a series of instabilities that play an important role in the formation of cardiac arrhythmias, like ventricular tachycardia. While the dynamics of single scroll waves have attracted some experimental effort, the interaction of scroll waves has so far received much less attention. We present an experimental study of the interaction of two scroll waves created in a Belousov-Zhabotinsky reaction medium and observed by optical tomography with a parallel beam technique. The scroll waves may either rotate in the same or in an opposite sense of rotation, thus leading to situations with different topological charges. The organising centres of the scrolls, the so-called filaments, were originally straight, and depending on the selected experimental conditions, they may either describe a circular or a meandering trajectory. The dynamics of pairs of co- and counter-rotating scroll waves were studied for both rigidly rotating and meandering filaments, leading to different types of collective filament behaviour.

(S01 – P7) Course of transient waves in weakly excitable media with application to spreading depolarization

Thomas M. Isele, Markus A. Dahlem

Institute for Theoretical Physics, Technical University of Berlin, Germany

We consider a modified model for an excitable medium where the homogeneous state is the only attractor. This model provides a phenomenological description for cortical spreading depolarization patterns. A variety of initial conditions is examined. These initial conditions are localized perturbations of the homogeneous state based on physiological grounds. We investigate the course of the resulting solutions. The emerging transient patterns and their classification according to size and duration offer insight into the pathophysiology of cortical spreading depression and migraine headache. The statistics of occurrences of the different classes has the potential to reproduce epidemiological statistics of different diagnostic forms of migraine such as migraine with or without headache.

(S01 – P8) Surfactant-induced gradients in Belousov-Zhabotinsky scroll waves

Dennis Kupitz[1], Sergio Alonso[2], Markus Bär[2], Marcus J. B. Hauser[1]

[1] Abt. Biophysik, Institut für Experimentelle Physik, Otto-von-Guericke-Universität Magdeburg, Universitätsplatz 2, 39106 Magdeburg, Germany, [2] Physikalisch-Technische Bundesanstalt, Berlin, Germany

Scroll waves are prominent patterns formed in three-dimensional excitable media, and they have been found to be at the basis of some types of cardiac arrhythmias. Experimentally, scroll waves dynamics is often studied by optical tomography in the Belousov-Zhabotinsky reaction, which produces CO_2 as an undesired product. Addition of small concentrations of a surfactant to the reaction medium is a popular method to suppress or retard CO_2 bubble formation. We report that in closed reactors even these low concentrations of surfactants are sufficient to generate vertical gradients of excitability, which are due to gradients in CO_2 and H^+ concentration. In reactors open to the atmosphere such gradients can be avoided. These gradients are shown to induce a twist onto vertically oriented scroll waves, while a twist is absent in scroll waves in a gradient-free medium. The effects of the CO_2 gradients are explained by a numerical study, where we modified the Oregonator model to account for the production of CO_2 and for its advection against the direction of gravity. The numerical simulations confirm the role of solubilized CO_2 as the source of the vertical gradients of excitability in reactors closed to the atmosphere.

(S01 – P9) Kinematic theory of spiral waves

M. Marmulla[1], *J. Löber*[1], *V. S. Zykov*[2], *H. Engel*[1]
[1] Institute for Theoretical Physics, Technical University of Berlin, [2] Max-Planck-Institute for Dynamics and Self-Organization, Göttingen

A universal kinematic description of rigidly rotating spiral waves [1] is applied to the Oregonator, Fenton-Karma and FitzHugh-Nagumo models to predict the rotation frequency as a function of the system parameters. The prediction is based on the measurements of the duration and the propagation velocity of an excitation pulse in a periodic wave train. The results are confirmed by direct numerical simulations of the underlying reaction-diffusion equations in two spatial dimensions. The computations are performed within broad parameter ranges of the reaction-diffusion models, where both rigidly rotating and meandering spiral waves are observed. Meandering is suppressed by a feedback-mediated control algorithm.

[1] V. S. Zykov. Kinematics of rigidly rotating spiral waves, *Physica D*, **238**, 931 (2008).

(S01 – P10) Complex patterns in fluid systems

Alberto P. Muñuzuri, Jacobo Guiu, Darío M. Escala, Alexandra von Kameke, Jorge Carballido-Landeira
Group of Nonlinear Physics, Fac. Fisicas, Univ. of Santiago de Compostela, 15782 Santiago de Compostela, Spain

Highly nonlinear mechanisms for pattern formation have been extensively studied due to the important role they play in Nature. The characteristic discrete nature of the biological systems (cellular compartment) has been recently analyzed. Nevertheless, many of these processes occur in a fluidic medium where hydrodynamic properties are especially relevant. Just no name a few examples; reactant pollutants dispersed in the atmosphere or in oceans; cells in living organisms are embedded in fluids, etc. We will present an analysis of the different properties characterizing the fluids on pattern formation. We consider typical pattern-forming reactions (Belousov-Zhabotinsky reaction like) with and without cell compartment but always in a liquid environment. Different instabilities are considered and the effect on the patterns observed analyzed. A first part of the contribution is devoted to the effect of external forcings on these systems. A well controlled turbulent flow can be generated that helps analyzing the effect of the different parameters on the patterning. Gravity modulations (Faraday type) among others will be considered in this context. A second part of the contribution considers gravity and density forces to be compatible with the propagation velocity of the patterns, so that interaction can be analyzed. Typical gravitational instabilities will be considered by changing viscosities and densities of the fluids under study. Experimental demonstrations of the different cases discussed will be shown and the results complemented and understood by theoretical and numerical analysis.

[1] G. Fernández-García, D. I. Roncaglia, V. Pérez-Villar, A. P. Muñuzuri, and V. Pérez-Muñuzuri. Chemical-wave dynamics in a vertically oscillating fluid layer. *Phys. Rev. E* **77**, 026204 (2008).
[2] A. von Kameke, F. Huhn, G. Fernández-García, A.P. Muñuzuri, and V. Pérez-Muñuzuri. Propagation of a Chemical Wave Front in a quasi two-dimensional Superdiffusive Flow. *Phys. Rev. E* **81**, 066211 (2010).
[3] J. Guiu-Souto, J. Carballido-Landeira, V. Pérez-Villar, and A. P. Muñuzuri. Manipulation of diffusion coefficients via periodic vertical forcing controls the mechanism of Turing pattern formation. *Phys. Rev. E* **82**, 066209 (2010).

(S01 – P11) Studying clock reactions in microflow

Robert Niedl, Igal Berenstein, Carsten Beta
Biological Physics, Institute of Physics and Astronomy, University of Potsdam

We study the dynamics of the autocatalytic iodate-arsenite reaction in PDMS-based microfluidic devices under continuous flow conditions. Two different scenarios are implemented to initiate the reaction. On the one hand, we use diffusive micromixing to systematically investigate the kinetics of the clock depending on the various input concentrations. On the other hand, we introduce a Pt electrode into the microchannel that acts as a local chemical source in the flow. This setup allows us to explore the interplay of flow velocity and source concentration that determines the initiation of this nonlinear reaction under flow conditions.

(S01 – P12) Evolution of a scroll ring in an oscillatory medium close to a Neumann boundary

Fabian Paul, Harald Engel
Institut für Theoretische Physik, TU Berlin, Hardenbergstraße 36, D-10623 Berlin

It is studied how the intrinsic dynamics of scroll rings in the complex Ginzburg-Landau equation [1] is affected by the presence of a Neumann boundary. For an untwisted scroll ring whose symmetry axis is oriented normally to the boundary, filament contraction is speeded up for cooperative setting while it is slowed down or even replaced by expansion for antagonistic setting. Numerically it is confirmed that boundary-induced drift, as studied in detail for two-dimensional spiral waves [2], is responsible for the observed changes in the growth rate. For an untwisted scroll ring with a symmetry axis inclined with respect to the Neumann boundary, the superposition of intrinsic and boundary-induced dynamics generates a phase shift along the filament eventually resulting in a helical instability [3,4].

[1] M. Gabbay, E. Ott, P. N. Guzdar, The dynamics of scroll wave filaments in the complex Ginzburg-Landau equation. *Physica D*, **118** (3-4), 371 (1998).
[2] I. S. Aranson, L. Kramer, A. Weber, Theory of interaction and bound states of spiral waves in oscillatory media. *Phys. Rev. E*, **47** (5), 3231 (1993).
[3] K. Nam, E. Ott, P. N. Guzdar, M. Gabbay, Stability of spiral wave vortex filaments with phase twists. *Phys. Rev. E*, **58** (2), 2580 (1998).
[4] G. Rousseau, H. Chate, R. Kapral, Twisted vortex filaments in the three-dimensional complex Ginzburg-Landau equation. *CHAOS*, **18** (2), 026103 (2008).

(S01 – P13) Pattern formation in the Belousov–Zhabotinsky-PAMAM dendrimer system

Diana I. Roncaglia[1], *Jorge Carballido-Landeira*[2] *and Alberto P. Muñuzuri*[2]
[1] Programa de Nanomedicinas, Universidad Nacional de Quilmes, Sáenz Peña 352 B1876BXD Bernal, Argentina, [2] Group of Nonlinear Physics, Univ. Santiago de Compostela, 15782 Santiago de Compostela, Spain

In this work, we present a new system using polyamidoamine (PAMAM) dendrimers on the Belousov-Zhabotinsky (BZ) reaction [1]. Dendrimers, so-called 'cascade molecules', have already found use as drug candidates for receptor–ligand interactions, drug carriers for conferring bio-survival, membrane permeability and targeting, and have found wide use as carriers for vaccine antigens as well. Dendritic structures are, despite their large molecular size, structurally well-defined, with a low polydispersity in comparison with traditional polymers. They are well-defined in both molecular weight and architecture and are capable of molecular inclusion, making ''unimolecular micelles'' [2,3]. The presence of dendrimers within the Belousov-Zhabotinsky reaction is systematically analyzed and the different macroscopic structures observed are reported [4]. First, the materials and setup used for this experimental study are described. The different structures observed and the effect of the dendrimer on the reaction is described within the context of pattern formation mechanisms.

[1] V. K. Vanag and I. R. Epstein, *Phys. Rev. Lett.*, **88**, 088303 (2002).
[2] J. L. Jackson, H. D. Chanzy, F. P. Booy, B. J. Drake, D. A. Tomalia, B. J. Bauer and E. J. Amis, *Macromolecules*, **31**, 6259 (1998).
[3] P. K. Maiti, T. Cagin, S. T. Lin and W. A. Goddard III, *Macromolecules*, **38**, 979–991 (2005).
[4] D. I. Roncaglia, J. Carballido-Landeira and A. P. Muñuzuri, *Phys. Chem. Chem. Phys.*, **13**, 7426–7432 (2011).

(S01 – P14) Pattern formation in halogen free reaction-diffusion systems

István Szalai[1], *Patrick De Kepper*[2] , *Judit Horváth*[1,2], *Nándor Takács*[1],
[1] Institute of Chemistry, Eötvös University, Budapest, Hungary, [2] CNRS Centre de Recherche Paul Pascal, Pessac, France

Many patterns in living and non-living systems result from the interplay of chemical and transport processes. In the studies of general aspects of reaction-diffusion systems, aqueous phase chemical systems are preferably used, since they are relatively easy to manipulate and the reactivity of reagents can be well controlled. However, sustained patterns were observed only in a limited domain of chemical compounds, namely that of the oxyhalogen oxidizing agents. Here, we report on halogen free reaction-diffusion systems, based on the hydrogen ion autocatalytic oxidation of sulfite ions by hydrogen-peroxide associated to two different types of proton consuming feedback reactions, which leads to sustained oscillatory spatiotemporal or stationary pH patterns. The stationary pattern formation requires restrained hydrogen ion diffusion. This is induced by the presence of suitable concentrations of polyelectrolyte species: These act as a reduced mobility buffers for hydrogen ions that affects both the effective reactivity and diffusivity of protons. These observations demonstrate that spatiotemporal patterns can be obtained experimentally in wider range of chemical systems.

(S01 – P15) Chemical pulses in biomimetic droplets

Jan Szymański[1], *Konrad Giżyński*[1], *Joanna Natalia Górecka*[2], *Jerzy Górecki*[1,3],
Klaus-Peter Zauner[4], Maurits de Planque[4]
[1] Institute of Physical Chemistry, Polish Academy of Sciences, Kasprzaka 44/52, 01-224 Warsaw, Poland, [2] Institute of Physics, Polish Academy of Sciences, Al. Lotnikow 36/42, 02-668 Warsaw, Poland, [3] Faculty of Mathematics and Natural Sciences, Cardinal Stefan Wyszynski University, Dewajtis 5, Warsaw, Poland, [4] School of Electronics and Computer Science, University of Southampton, UK

We demonstrate that aqueous droplets of the diameter on the order of 1 mm containing the Belousov-Zhabotinsky reaction reagents are capable of sustaining chemical waves. The droplets are surrounded by solution of phospholipids in decane and are therefore stabilized by lipid monolayers. When the droplets are forced into close contact they synchronize through the resulting bilayers – the chemical pulses are transmitted from one droplet to another, adjacent one. Varying the excitability and the diameters of neighboring droplets we observe changes in pulse frequency between droplets and onset of the diode action, whereby pulses move from bigger to smaller droplets, but not the other way around. We present a preliminary numerical model that quantitatively describes the relation between the chemical composition of the droplets and the pulse frequency.

(S01 – P16) Pattern formation in the hydrogen peroxide-sulfite-ferrocyanide reaction

Nándor Takács[1], *Patrick De Kepper*[2], *Judit Horváth*[1,2], *István Szalai*[1]
[1] Institute of Chemistry, Eötvös University, Budapest, Hungary, [2] CNRS Centre de Recherche Paul Pascal, Pessac, France

The hydrogen-peroxide-sulfite-ferrocyanide (HPSF) system is a pH-oscillator that shows bistability and temporal pH-oscillations in a continuous stirred-tank reactor. [1] Here we present systematic studies of the spatiotemporal dynamics of the HPSF reaction in open gel reactors. To explore the pattern forming capacity of the HPFS system we followed our previously proposed systematic method. [2] As a result spatial bistability, traveling waves and stationary patterns were obtained. Furthermore, peculiar spatiotemporal phenomena, e.g. transition from an oscillatory to a spatially homogenous state trough spatially damped oscillations, and formation of stationary stripes through spatiotemporal oscillations were observed. These are the sign of a bistability which can be the result of a subcritical bifurcation. The effect of some important experimental parameters e.g. the thickness of the gel and the boundary geometry are presented.

[1] G. Rabai, K. Kustin, I. R. Epstein, A systematically designed pH oscillator: the hydrogen peroxide-sulfite-ferrocyanide reaction in a continuous stirred tank reactor. *J. Am. Chem. Soc.,* **111**, 3870 (1989).
[2] J. Horváth, I. Szalai, P. De Kepper, An experimental design method leading to chemical Turing patterns. *Science*, **324**, 772 (2009).

(S01 – P17) Superstructures and chirality reversal in the media of homoclinic oscillations

Xiaodong Tang[1], *Qingyu Gao*[1], *Shirui Gong*[1], *I. R. Epstein*[2]
[1] College of Chemical Engineering, China University of Mining and Technology, Xuzhou 221008 China, [2] Department of Chemistry and Volen Center for Complex Systems, MS 015, Brandeis University, Waltham, Massachusetts 02454-9110, USA

Compared with the significant progress that has been achieved in excitable, simple and period-doubled oscillatory media [1, 2], considerably less is known about patterns in media that supports local homoclinic oscillations [3]. We seek here to study the pattern formation of a three-variable reaction-diffusion model with two positive feedbacks, which support mixed-mode oscillations. And we find in 1-D system, the model may display a kind of traveling waves with periodic amplitude modulation. A new wave with small peak can be generated on one side of the traveling waves when the amplitude reached its maximum and disappeared at the minimum amplitude of the waves from amplitude offset. We have a hypothesis that the two waves may have periodic interaction with each other during the waves traveling, which cause the amplitude modulation. All of the traveling waves in this system repeat this modulation period with spatial phase difference. So the whole system may exhibit a type of super-structure: super-traveling waves, which displays like a bigger traveling wave constructed by the basic modulated traveling waves. We also do some numerical simulation of this model in 2-D system, which generated spiral waves with amplitude modulated spiral arms. This results in a variety of spatiotemporal patterns such as supertargets (circular waves superimposed on spiral waves [4]), superspirals, and line-defect spirals in numerical simulations of the same reaction-diffusion model. Variation of a control parameter can reverse the chirality of superspiral patterns too. These amplitude-modulated patterns may provide insights into mechanisms of pattern development in some living systems.

[1] A. Goryachev, H. Chate & R. Kapral, *Phys. Rev. Lett.* **80**, 873 (1998).
[2] J. S. Park, S. J. Woo & K. J. Lee, *Phys. Rev. Lett.* **93**, 098302 (2004).
[3] Qingyu Gao, Lu Zhang, Qun Wang, and I. R. Epstein, *CHAOS* **19**, 013135 (2009).
[4] L. Zhang, Q. Y. Gao, Q. Wang & J. Wang, *Phys. Rev. E* **74**, 046112 (2006).

(S01 – P18) A discrete model to study reaction-diffusion-mechanics systems

Louis D. Weise[1], *Martyn P. Nash*[2], *Alexander V. Panfilov*[3]
[1] Department of Theoretical Biology, Utrecht University, Utrecht, The Netherlands, [2] Auckland Bioengineering Institute and Department of Engineering Science, The University of Auckland, New Zealand, [3] Department of Physics and Astronomy, Ghent University, Ghent, Belgium

A discrete reaction-diffusion-mechanics (dRDM) model has been developed to study the effects of deformation on wave propagation in excitable media. The dRDM framework couples a FitzHugh-Nagumo type reaction-diffusion model for cardiac excitation to a finite elastic mass-lattice model. The dRDM framework is shown to be computationally efficient, and to reproduce previously found effects [1] on self-organised pacemakers. With the dRDM approach new mechanisms that determine the period and drift of pacemakers were identified. The dRDM model could be applied to other excitable media and extended to large systems such as whole-heart models.

[1] A. Panfilov, R. Keldermann, M. Nash, Self-organised pacemakers in a coupled reaction-diffusion-mechanics system, *Phys. Rev. Lett.*, **95**, 25 (2005).

Symposium 2: **Reactive Gels**

(S02 – I) Introduction

Irving R. Epstein

Department of Chemistry, MS 015, Brandeis University, Waltham, MA 02454, USA

The earliest studies of pattern formation in reaction-diffusion systems took place in aqueous solution or on solid surfaces. Complex media like membranes or microemulsions can give rise to an even richer variety of patterns and more closely approximate the structure of biological systems. Among such complex media, reactive gels are of particular interest, particularly because they offer the possibility of coupling chemical change to mechanical motion, as occurs in nearly all living organisms. This mini-symposium will explore recent progress, both experimental and theoretical, in studying reactive gels.

(S02 – T1) Self-oscillating polymer gels as smart materials

Ryo Yoshida

Department of Materials Engineering, Graduate School of Engineering, The University of Tokyo, Japan

So far stimuli-responsive polymer gels and their application to smart materials have been widely studied. On the other hand, as a novel biomimetic gel, we have been studying gels with an autonomous self-oscillating function, since firstly reported in 1996 [1,2]. We succeeded in developing novel self-oscillating polymers and gels by utilizing the oscillating reaction, called the Belousov-Zhabotinsky (BZ) reaction. The self-oscillating polymer is composed of a poly(N-isopropylacrylamide) network in which the catalyst for the BZ reaction is covalently immobilized. In the presence of the reactants, the polymer gel undergoes spontaneous cyclic swelling–deswelling changes or soluble–insoluble changes (in the case of uncrosslinked polymer) without any on–off switching of external stimuli. Potential applications of the self-oscillating polymers and gels include several kinds of functional material systems, such as biomimetic actuators and mass transport surface.

[1] R. Yoshida, T. Takahashi, T. Yamaguchi and H. Ichijo, *J. Am. Chem. Soc.*, **118**, 5134 (1996).

[2] R. Yoshida, *Adv. Mater.*, **22**, 3463 (2010).; *Polym. J.*, **42**, 777 (2010).

(S02 – T2) Rational experimental construction of chemomechanical oscillators with non-oscillatory reactions

Judit Horváth[1,2], *István Szalai*[1], *Patrick De Kepper*[2]

[1] Institute of Chemistry, Eötvös Loránd University, Budapest, Hungary,[2] CNRS Centre de Recherche Paul Pascal, Bordeaux, France

A first partial demonstration of Jacques Boissonade's theoretical prediction had been realized with the supercatalytic chlorite-tetrathionate reaction in 2005. However, only chemomechanical excitability waves were clearly identified in that system. We now provide demonstration of well-identified chemomechanical oscillations in two new acid autocatalytic systems: In the bromate-sulfite reaction the system was shown to produce a dozen of swelling-shrinking cycles and to work under mechanical stress. The lifetime of this system was limited due to bromination side-reactions of the gel matrix. This degradation does not occur in the iodate-sulfite (Landolt) reaction where oscillations could be maintained for more than a week with no damping. These results were obtained by rational adjustment of the gel properties to the position and amplitude of the pH-drop in the clock reaction. We shall discuss what are the clue elements to assemble such type of oscillators. We will show how this reasoning could be extended to further pH and other responsive materials.

[1] J. Horváth, I. Szalai, J. Boissonade, P. De Kepper, Oscillatory dynamics induced in a responsive gel by a non-oscillatory chemical reaction: experimental evidence, *Soft Matter*, accepted.

(S02 – T3) Responsive supramolecular hydrogels for chemomechanical systems

Ye Zhang [1], *Jorge Delgado* [1], *Ning Li* [2], *Irving R. Epstein* [1] *and Bing Xu* [1]

[1] Department of Chemistry, [2] Department of Physics, Brandeis University, Waltham, MA 02454, USA

Inspired by the natural materials that convert chemical energy into mechanical movement, we designed and fabricated chemomechanical hydrogels. In this talk, we will discuss a new type of supramolecular hydrogels that may offer a new system for exploring chemomechanical hydrogels. By using Belousov-Zhabotinsky (BZ) oscillating chemical reaction as theoretical modeling, we built the catalyst of BZ reaction-ruthenium complex into a copolymer or a supramolecular gelator to form hydrogels. The periodic oxidation and reduction of the anchored ruthenium ion in BZ reaction induce the corresponded hydrating and dehydrating effects in the hydrogels that finally result into its oscillatory volume change. In addition, we will also discuss the phase-transition of supramolecular hydrogels upon enzymatic catalysis. The overall aim of our research is to explore the possibility of utilizing hererogeneous chemoresponsive gels to produce multifunctional materials with the ability to convert the chemical energy of an oscillating chemical reaction into controllable mechanical forces.

[1] Delgado, J.; Zhang, Y.; Xu, B.; Epstein, I. R. “Terpyridine- and Bipyridine-based Ruthenium Complexes as Catalysts for the Belousov-Zhabotinsky Reaction” *J. Phys. Chem. A*, **115**, 2208 (2011).

[2] Yang, Z. M.; Liang, G. L.; Xu, B. “Enzymatic hydrogelation of small molecules” *Acc. Chem. Res.*, **41**, 315 (2008).

(S02 – T4) Computational design of active, self-reinforcing gels

Victor V. Yashin, Olga Kuksenok, Anna C. Balazs
Chemical Engineering Department, University of Pittsburgh, Pittsburgh, PA 15261, USA

Many living organisms have evolved a protective mechanism that allows them to reversibly alter their stiffness in response to mechanical contact. Using theoretical modeling, we design a mechanoresponsive polymer gel that exhibits a similar self-reinforcing behavior. We focus on cross-linked gels that contain Ru(terpy)$_2$ units, where both terpyridine ligands are grafted to the chains. The Ru(terpy)$_2$ complex forms additional, chemoresponsive cross-links that break and re-form in response to a repeated oxidation and reduction of the Ru. In our model, the periodic redox variations of the anchored metal ion are generated by the Belousov-Zhabotinsky (BZ) reaction. Our computer simulations reveal that compression of the BZ gel leads to a stiffening of the sample due to an increase in the cross-link density. These findings provide guidelines for designing biomimetic, active coatings that send out a signal when the system is impacted and use this signaling process to initiate the self-protecting behavior.

(S02 – P1) Modeling contraction patterns in protoplasmic droplets of *Physarum polycephalum*

Markus Radszuweit[1], Harald Engel[2] and Markus Bär[1]
[1] Physikalisch-Technische Bundesanstalt, Berlin, [2] Institut für Theoretische Physik, TU Berlin

Protoplasmic droplets of the slime mold *Physarum polycephalum* develop various contraction patterns during their development. We present a model of these droplets that incorporates the important chemical and mechanical aspects of the cell in a physiological realistic way. To account for the cell mechanics we consider the protoplasm as a two-phase incompressible medium consisting of an active elastic gel and a fluid sol phase. We write the elastic equations for the gel, describing the dynamics of deformations, and a hydrodynamic equation for the sol in a regime of large Reynolds numbers. A calcium oscillator whose dynamics is governed by a reaction-diffusion-advection equation generates the mechanical stresses. For small deformations an approximative model involving global coupling was derived and analyzed [1]. Numerical simulations using the FEM technique in one and two dimensions are performed and confirm the theoretical predictions. Furthermore simulations of the full model are compared with experimentally observed spatiotemporal contraction patterns. For certain cases we find a qualitative agreement between the patterns of the model and the experimental results.

[1] "A model for oscillations and pattern formation in protoplasmic droplets of Physarum polycephalum", *Eur. Phys. J. Special Topics,* **191,** 159–172 (2010).

Symposium 3: **Chemical Oscillators**

(S03 – I) Introduction

Jürgen Kurths
Potsdam Institute for Climate Impact Research, Germany

(S03 – T1) Kinetic switches with catalytic particles coupled by chemical exchange

Annette F. Taylor[1], Mark Tinsley[2], F. Wang[2], Ken Showalter[2]
[1] School of Chemistry, University of Leeds, UK, [2] Department of Chemistry, West Virginia University, USA

Cellular biological systems such as yeast cells and bacteria communicate via chemicals emitted into an extracellular solution. This global signal is used to synchronise the activity of the population but can also divide the cells into sub-groups in different chemical states. When the signal contains feedback in the kinetics then sharp transitions between states can be observed as a function of some parameter such as the cell density. We used [1, 2] catalytic particles suspended in catalyst-free Belousov-Zhabotinsky (BZ) solution to investigate the driving forces behind these kinetic switches. Simulations provided insight into the experimental results and allowed us to design systems displaying particular states, depending on the type of catalyst used and the density of particles.

[1] A.F. Taylor, M.R. Tinsley, F. Wang, Z. Huang, K. Showalter, *Science*, **323**, 614-617 (2009).
[2] A.F. Taylor, M.R. Tinsley, F. Wang, K. Showalter, *Angew. Chem. Int. Ed.*, **50**, (2011).

(S03 – T2) Synchronization of small networks of electrochemical oscillators

István Z. Kiss, Mahesh Wickramasinghe, Emily Mrugacz
Department of Chemistry, Saint Louis University, St Louis, MO 63103, USA

Experiments are carried out with small networks of periodic and phase coherent chaotic oscillators obtained with a chemical system of nickel electrodissolution in sulfuric acid. A hybrid chemical-resistor system is built in which network topology can be induced with cross resistors placed between the electrodes. Transition to identical synchronization occurred at critical coupling strengths that strongly varied with the number of chaotic oscillators (2-4) and the coupling topology; the critical coupling strength was found to be inversely proportional to the second largest eigenvalue of the connectivity matrix, i.e., the experiments confirm the Wu-Chua conjecture [1]. In the weakly coupled chaotic phase synchronized state we show that the coupling topology can deduced from dynamical measurements using bivariant and partial phase synchronization indices [2]. Finally, anomalous phase synchronization effects [3] of asymmetrical coupling induced by size disparity between the electrodes are described with a pair of periodic oscillators. The experiments show that the dynamical behavior of the chemical oscillator assembly can be effectively tuned with designed coupling structure and symmetry.

[1] C. W. Wu and L. O. Chua, *IEEE Trans. Circuits Syst.-I*, **43**, 161 (1996).
[2] B. Schelter et al., *Phys. Rev. Lett.*, **96**, 208103 (2006).
[3] B. Blasius, *Phys. Rev. E*, **72**, 066216 (2005).

(S03 – T3) Oscillation quenching mechanisms: amplitude vs. oscillation death

Aneta Koseska[1], *Evgenii Volkov*[2], *Jürgen Kurths*[3,4]
[1] Interdisciplinary Center for Dynamics of Complex Systems, University of Potsdam, [2] Lebedev Physical Institute, Moscow, Russia, [3] Potsdam Institute for Climate Impact Research, Potsdam, Germany, [4] Institute of Physics, Humboldt University, Berlin, Germany

Coupled oscillators constitute an effective and popular paradigm for the study of interacting oscillatory processes in the physical, chemical and biological sciences. Despite various rhythmogenic activity which can occur in coupled system (e.g. synchronization, as one of the most studied phenomena), special attention has also been paid to the suppression of oscillations, whereby individual oscillators cease to oscillate when coupled and go to one or more equilibrium solutions. Here we study two main manifestations of oscillation quenching - amplitude and oscillation death phenomena, giving an overview on the background of emergence of both manifestations. Moreover, we demonstrate a novel effect: under strong coupling via slow variable, detuning can eliminate standard oscillatory solutions from a large region of the parameter space, establishing the dominance of oscillation death. The results are further related to Turing structures and their interpretation in multicellular systems.

(S03 – T4) Synchronisation of chemical oscillators undergoing the Belousov-Zhabotinsky reaction

Claudia Lenk[1], *Philipp Maass*[2], *and Michael Köhler*[1]
[1] Institut für Physik, Technische Universität Ilmenau, 98684 Ilmenau, Germany, [2] Fachbereich Physik, Universität Osnabrück, 49076 Osnabrück, Germany

Propagating chemical waves in the Belousov-Zhabotinsky reaction are in close resemblance to excitation patterns observed in various biological media as, for example, the mammalian heart tissue or animal retinas. It has been argued in the literature that the cellular nature of these biological systems plays an important role for the occurring wave patterns. In order to get insight into the effects of the cellular nature we study influence of different spatial inhomogeneous catalyst distributions on the excitation patterns of the Belousov-Zhabotinsky reaction in a silica gel. Arrays of catalyst spots are generated in this silica gel or a Nafion membrane and the synchronisation between the oscillations of the single spots is analysed in dependence of the spot size and spot distance. In addition the influence of gradual changes of the spot distance and size inside the spot array pattern is studied. Our results are compared to numerical findings from calculations of the FitzHugh-Nagumo equations.

(S03 – T5) Chemical oscillators involving noble Metal nanoparticles

István Lagzi[1], *Bartlomiej Kowalczyk*[2], *Dawei Wang*[3], *Bartosz A. Grzybowski*[2]
[1] Department of Meteorology, Eötvös University, [2] Department of Chemistry, Northwestern University, [3] School of Materials Science and Engineering, Northwestern Polytechnical University

Chemical oscillations are important in many biological processes and are relevant to fundamental research on non-linear chemical phenomena. We demonstrate that chemical oscillators operating at molecular scales can be coupled to nanoscopic components and can drive their reversible assembly [1]. Periodic pH changes translate into protonation and deprotonation of ligands stabilizing metal nanoparticles (NP) and alter the subtle balance between the repulsive electrostatic and attractive van der Waals interparticle forces. In a continuously stirred reactor, these changes give rise to rhythmic aggregation and dispersion of the NPs. The ability to engineer non-linear behaviors into nanoscale systems can open new vistas to stimuli-responsive, dynamic nanomaterials.

[1] I. Lagzi, B. Kowalczyk, D. Wang, B. A. Grzybowski. Nanoparticle oscillations and fronts, *Angew. Chem. Int. Ed.*, **49**, 8616 (2010).

(S03 – P1) Evidence of chemical oscillations in the sodiuborohydride hydrolysis

Marcello A. Budroni[1], *Emiliano Biosa*[2], *Sebastiano Garroni*[2], *Gabriele Mulas*[2], *Nadia Marchettini*[1], *Mauro Rustici*[2]
[1] Department of Chemistry, University of Siena, Italy, [2] Department of Chemistry, University of Sassari, Italy

Studying hydrogen as an alternative source of energy is a transversal and challenging topic in science. In this context the hydrolysis of sodium borohydride represents one of the most promising processes through which highly pure hydrogen can be generated. The apparent simplicity of this reaction and the significant quantity of hydrogen $NaBH_4$ can release make it an optimal candidate for devices able to transform hydrogen into energy. Here we discuss the first experimental evidence that the sodium borohydride hydrolysis is a chemical oscillator. This is of primary importance from both a theoretical point of view and from an applicative perspective since understanding nonlinear phenomena can be fundamental for the chemical control of the process and for the optimization of hydrogen devices.

(S03 – P2) Synchronization and its breakdown in mobile oscillator networks

Naoya Fujiwara[1], *Jürgen Kurths*[1,2], *Albert Díaz-Guilera*[3,1]
[1]Potsdam Institute for Climate Impact Research, Germany, [2]Institute for Complex Systems and Mathematical Biology, University of Aberdeen, UK, [3]Departament de Física Fonamental, Universitat de Barcelona, Spain

We present a model of synchronization in mobile networks of autonomous agents where the topology changes due to agents motion. We present that there exist two distinct timescales, one for the topological change and another one for local synchronization. We observed two different mechanisms leading to synchronization depending on the dominant time scale [1]. We introduce an analytical procedure by means of spectral analysis of the time-dependent Laplacian matrix. Moreover, we show that the breakdown of synchronization takes place in chaotic systems.

[1] N. Fujiwara, J. Kurth, and A. Díaz-Guilera, *Phys. Rev. E* **83,** 025101(R) (2011).

(S03 – P3) Optimal phase response curves for stochastic synchronization of limit-cycle oscillators by common Poisson noise

Shigefumi Hata[1], *Hiroya Nakao*[2]
[1] Department of Physics, Kyoto University, Kyoto, Japan, [2] Department of Mechanical and Environmental Informatics, Tokyo Institute of Technology, Tokyo, Japan

Optimization of phase response curves (PRCs) for stochastic synchronization induced by common Poisson noise is considered. The Lyapunov exponent, which quantifies the linear stability of the synchronization, is given as a functional of the PRC [1][2]. By solving the Euler-Lagrange equation, we calculate the PRCs with which the Lyapunov exponent takes the minimum. We show that the optimal PRC for stochastic synchronization mutates from a sinusoid to a sawtooth by increasing its squared oscillators with the optimal PRCs.

[1] K. Arai and H. Nakao, *Phys. Rev. E* **78**, 066220 (1-8) (2008).
[2] S. Hata, T. Shimokawa, K. Arai and H. Nakao, *Phys. Rev. E* **82**, 036206 (1-12) (2010).

(S03 – P4) Synchronization and bulk oscillations in auto-catalytic reactions

Nikos Kouvaris[1,2], *Dimitris Kugiumtzis*[2], *Astero Provata*[1]
[1] Institute of Physical Chemistry, National Center for Scientific Research "Demokritos", Athens, Greece, [2] Department of Mathematical, Physical and Computational Science, Aristotle University of Thessaloniki, Greece

A prototype auto-catalytic reaction model with cyclic domination of four species and empty sites is proposed for studying transition to synchronization. At the mean field level the dynamics shows quasi-periodicity and chaos depending on the parameter values. The realization of the model on a square lattice shows that spacial restrictions and intrinsic stochasticity change the whole picture. The mean field dynamics qualitatively remains only under global reactions, while local reactions drive the lattice to poisoning. Non-trivial oscillatory steady states are developed if long distance exchange is introduced due to gradual mixing with a certain probability. The mixing probability is shown to control the transition to synchronization which emerge abruptly following a phase slip scenario. Near the transition a typical intermittency crisis takes place with phase slips becoming more infrequent as the transition is approached.

[1] B. Blasius, A. Huppert and L. Stone, *Nature* **399**, 354-359 (1999).
[2] T. Reichenbach, M. Mobilia and E. Frey, J. Theor. Biol. **254**, 368-383 (2008).
[3] N. Kouvaris, A. Provata and D. Kugiumtzis, Phys. Lett. A **374**, 507-515 (2010).

(S03 – P5) Generation of pH-oscillations in closed chemical systems: Method and applications

Eszter Poros,[†] *Viktor Horváth,*[†] *Krisztina Kurin-Csörgei,*[†] *Irving R. Epstein*[‡*] *and Miklós Orbán*[†*]
Department of Analytical Chemistry, L. Eötvös University, H-1518 Budapest 112, P.O. Box 32, Hungary, and Department of Chemistry and Volen Center for Complex Systems, MS 015, Brandeis University, Waltham, Massachusetts 02454-9110, USA

Along with the BrO_3^- and ClO_2^- oscillatory systems, the pH-oscillators represent the group that has been most frequently employed to study nonlinear chemical dynamics and it is this group that offers the greatest promise for practical applications. All pH-oscillators known to date function only under flow conditions (in a CSTR or semibatch arrangement). In several proposed applications a batch pH-oscillator would be more convenient and practical to use than the equivalent flow variant. In this poster we show an approach to generating pH-oscillations in a closed system by starting from an open system pH-oscillator, finding semibatch condiditions under which it oscillates with an inflow of a single reactant to an otherwise closed reactor containing the remaining components, and replacing this inflow with a layer of silica gel impregnated with the key reactant. The successful application of the technique is demonstrated to generate long lasting batch pH-oscillations in the $BrO_3^- - Mn^{2+} - SO_3^{2-}$, $IO_3^- - Fe(CN)_6^{4-} - SO_3^{2-}$ and $BrO_3^- - Fe(CN)_6^{4-} - SO_3^{2-}$systems.

(S03 – P6) Origin of reliable time in biological clocks: Theoretical approach using coupled phase oscillators

Fumito Mori[1], *Hiroshi Kori*[1,2]
[1] Division of Advanced Sciences, Ochanomizu University, Tokyo, Japan,[2] PRESTO, Japan Science and Technology Agency, Kawaguchi, Japan

Biological rhythms, such as circadian rhythms and heartbeats, are noted for their temporally precise oscillations. Herzog *et al.* observed circadian rhythms in mice kept in dark room, and found that the standard deviation of circadian periods

between the onsets of activity is smaller than that between the offsets [1]: onset time in the circadian activity kept by a biological clock seems to be more reliable than offset time. Motivated by this observation, using a coupled phase oscillator model with noise, we investigate how and why the reliability of time varies within one cycle. We theoretically show that such variation is associated with the interaction between oscillators.
[1] E. D. Herzog, S. J. Aton, R. Numano, Y. Sakaki and H. Tei, *J. Biol. Rhythms,* **19**, 35 (2004).

(S03 – P7) Modeling studies of the oscillatory phenylacetylene carbonylation reaction

Katarina Novakovic

School of Chemical Engineering and Advanced Materials, Newcastle University, UK

The palladium-catalysed phenylacetylene oxidative carbonylation (PCPOC) reaction exibits oscilations in pH, as well as heat of reaction (Qr), when operating in a stirred batch reactor [1-2]. When running in an oscillatory regime high levels of product selectivity are reported compared to a non-oscillatory mode [2]. The aforementioned imply the need for a fundamental understanding of the PCPOC reaction. Previous experimental and modelling studies revealed the significant role played by traces of water contained in the standard HPLC grade methanol used [3]. In this paper further developments of a reaction network responsible for the oscillatory nature of the PCPOC reaction are reported.
[1] K. Novakovic, C. Grosjean, S. K. Scott, A. Whiting, M. J. Willis, A. R. Wright, Achieving pH and Qr oscillations in a palladium catalysed phenylacetylene oxidative carbonylation reaction using an automated reactor system, *Chem. Phys. Lett.*, **435**, 142 (2007).
[2] K. Novakovic, C. Grosjean, S. K. Scott, A. Whiting, M. J. Willis, A. R. Wright, The influence of oscillations on product selectivity during the palladium-catalysed phenylacetylene oxidative carbonylation reaction, *PCCP*, **10**, 749 (2008).
[3] K. Novakovic, J. Parker, Catalyst initiation in the oscillatory carbonylation reaction, *Int. J. Chem. Eng.*, in press.

(S03 – P8) Control of spontaneous spirals formation in a zwitterionic micellar medium

Federico Rossi[1], Rosario Varsalona[2], Nadia Marchettini[1], Maria Liria Turco Liveri[2]

[1] Department of Chemistry, University of Siena, Italy,[2] Department of Chemistry, University of Palermo, Italy

The transition from planar fronts, trigger waves or solitary pulses to spirals in excitable media attracted an increasing interest in the past few decades, mainly because of its relevance for biological and medical applications. In this contribute we describe a new and convenient method for spirals generation starting from symmet- ric wavefronts. By using the micelle-forming zwitterionic surfactant *N*-tetradecyl- *N,N*-dimethylamine oxide in a Belousov-Zhabotinsky solution, it is possible to control to a large extent the domains where spirals can be spontaneously generated. The mechanism responsible for the wavefront break up lies on the interaction of the propagating waves with the unexcitable regions formed by the interaction of the micelles with some of the Belousov-Zhabotinsky key intermediates.

(S03 – P9) Autocatalytic reaction and flow in porous media: an active tracer

Séverine Atis, Harold Auradou, Laurent Talon and Dominique Salin

Universités Pierre et Marie Curie, Paris Sud and CNRS; Laboratoire FAST, Bâtiment 502, UPS, 91405 Orsay Cedex, France

Coupling between autocatalytic reaction front and simple hydrodynamic flows leads to front patterns revealing the underlying flow field [1]. Flow of a passive tracer, i. e. a dye, through the complex flow field of a porous medium leads to the so-called hydrodynamic dispersion which accounts for the mixing process inside the medium [2]. We have performed experiments and numerical simulations of the propagation of reaction front in a heterogeneous porous medium. We have analyzed the dependence of the shape and velocity of the front with the flow rate and heterogeneity intensity. As a result this active, chemical, tracer allows to access to the characteristic of the complex flow field of the porous medium.
[1] M. Leconte, J. Martin, N. Rakotomalala and D. Salin. Pattern of reaction diffusion front in laminar flow. *Phys. Rev. Lett.*, **90** , 128302 (2003).
[2] J. C. Bacri, N. Rakotomalala and D. Salin. Experimental evidence of disorder effects in hydrodynamic dispersion. *Phys. Rev. Lett.*, **58,** 2035 (1987).

(S03 – P10) Synchronization of noisy oscillators

Ralf Toenjes, Hiroshi Kori

Academic Production, Ochanomizu University, Tokyo, Japan

Adopting the very general picture of a noisy oscillator as a closed, stochastic dynamical system with nonzero stationary flows we use Markov chains to model synchronization of such systems. We are in particular interested in the change of the mean frequency and the coherence of the stochastic oscillations in response to the frequency of a driving signal. If the transition rates are perturbed weakly, perturbation theory can predict the frequency change very well. Our work demonstrates how synchronization extends to systems with strong noise and complex attractors as opposed to weakly noise perturbed limit cycle oscillators. We will discuss possible applications such as control of molecular machines and optimization in stochastic transport networks.

(S03 – P11) Exploring feedback in enzymatic systems

Magdalena M. Wrobel[1], *Annette F. Taylor*[1], *Stephen K. Scott*[1], *John A. Pojman*[2]
[1] School of Chemistry, University of Leeds, United Kingdom, [2] Department of Chemistry, Louisiana State University, Baton Rouge, Louisiana, United States

Feedback is widely spread in biological and chemical systems leading to interesting effects as clocks, fronts, bistability and oscillations. Enzymatic systems are also expected to exhibit complex behavior as positive feedback is present through coupling acid/base production with the bell-shaped dependence of enzyme activity on pH [1]. A new experimental example of the effects of feedback in enzymatic systems is the urea-urease reaction that shows clocks in batch, bistability in flow [2] and fronts in spatial system. This reaction is a good candidate to show oscillations when coupled with a source of negative feedback.

[1] Shen P., Larter R., Role of substrate inhibition kinetics in enzymatic chemical oscillations, *Biophys. J.*, **4**, 67 (1994),
[2] Hu, G.; Pojman, J. A.; Scott, S. K.; Wrobel, M. M.; Taylor, A. F., Base catalyzed feedback in the urea-urease reaction, *J. Phys. Chem. B*, **44**, 114, (2010).

Symposium 4: **Single Molecule Imaging and Manipulation**

(S04 – I) Introduction

Leonhard Grill
Department of Physical Chemistry, Fritz Haber Institute of the MPG, Berlin

Scanning probe microscopy (SPM) techniques, invented in the 1980-ies, are very powerful methods to study matter at the atomic scale as has been shown in the last decades by many studies. In the last 10-20 years, intense research was done on the investigation of single molecules on surfaces as SPM does not only allow to image them with submolecular resolution, but also to manipulate them in a controlled way. The latter is of high interest to trigger and thus study specific functions that are incorporated in the molecules. The local probing approach plays an important role, because it gives direct insight into the molecular response on the external stimulus and allows also to characterize and thus consider the atomic-scale environment of the molecule, which can play an important role for the specific function. In this presentation, an introduction into the field of single molecule manipulation will be given by several examples from the last years.

(S04 – T1) Scanning tunneling/atomic force microscopy of individual atoms/molecules on insulating films

Gerhard Meyer[1], *Leo Gross*[1], *Fabian Mohn*[1], *Nicolaj Moll*[1], *Peter Liljeroth*[2] *and Jascha Repp*[3]
[1] IBM Research - Zurich, Rüschlikon, Switzerland, [2] Department of Applied Physics, Aalto University School of Science, Finland, [3] Institute of Experimental and Applied Physics, University of Regensburg, Germany

Ultrathin insulating films on metal substrates are unique systems to use the Scanning Tunneling / Atomic Force Microscope to study the electronic and structural properties of single atoms and molecules, which are electronically decoupled from the metallic substrate. For example individual metal atoms on an ultrathin insulating film exhibit different charge states, which are stabilized by the large ionic polarizability of the film. In the case of molecules the electronic decoupling allows the imaging and manipulation of molecular orbitals. As we have recently demonstrated, detailed structural information can be attained by Atomic Force Microscopy, which leads to the direct imaging of the molecular geometry. The complete chemical structure of single molecules can be accessed in scanning probe microscopy [1].

[1] L. Gross, F. Mohn, N. Moll, P. Liljeroth, G. Meyer, The Chemical Structure of a Molecule Resolved by Atomic Force Microscopy, *Science,* **325**, 1110-1114 (2009).

(S04 – T2) Molecular organization on surfaces studied by UHV-STM: Reaction, chirality and dynamics

Trolle Rene Linderoth
Interdisciplinary Nanoscience Center (iNANO) and Department of Physics and Astronomy, Aarhus University, Denmark

In the on-surface synthesis scheme for forming molecular nanostructures on surfaces, the molecular building blocks are joined by covalent bonds, which are anticipated to provide increased thermal and chemical stability compared to conventional non-covalent self-assembly. Considerable attention has recently been devoted to this approach, and I will review work where we have explored a two-component condensation reaction between aldehyde and amine compounds performed under UHV conditions on a Au(111) surface to form reaction products joined by imine-bonds [1]. The combination of on-surface synthesis and subsequent self-assembly can provide unique structures that are not obtained by conventional, direct deposition of similar molecular building blocks. Two-dimensional branched polymeric surface networks and nanoscopic pores are obtained using three-spoke aldehydes and di-amine linkers, and it is demonstrated that the network connectivity can be controlled by varying kinetic parameters of the preparation procedure. The second part of the talk will concern chiral self-assembly on surfaces [2]. We recently identified a novel mechanism of chiral switching which occurs by spontaneous conformational changes in a rod-shaped compound equipped with bulky side-groups. By investigating an entire class of related compounds with systematically varied chemical functionality of their terminal groups we demonstrate we can control both the conformational chirality of the individual molecules and the organizational chirality in surface assemblies resulting from them. Most recently, we have used an intrinsically chiral member of this class of compounds to form globally homochiral assemblies and control the chirality of assemblies from non-chiral molecules through chiral induction.

[1] *Angew. Chem.* **46,** 9227 (2007), **47,** 4406 (2008), *ACS NANO* **2,** 651 (2008).
[2] *Nat. Mat.* **5,** 11 (2006), *ACS NANO* **4,** 297 (2010), *JACS* **133,** 4896 (2011).

(S04 – T3) Spectroscopic signature of single Au(III) porphyrin cations on a gold surface

Stefan Müllegger, Mohammad Rashidi and Reinhold Koch
Institute of Semiconductor and Solid State Physics, Johannes Kepler University Linz, Austria

The stabilization of charged functional molecules on a supporting surface requires appropriate coupling to their surroundings. Recently, we investigated the adsorption of single Au(III) porphyrin molecules on a gold surface observing only weak effects on the frontier orbital energy levels compared to solution [1] as well as a rich variety of structural conformers. [2] Here, we employ low-temperature (LT) scanning tunneling microscopy (STM) and - spectroscopy (STS) to study substrate-induced effects on the metal-ligand bonding interaction of phenyl-substituted Au(III) porphyrin cations on a Au(111) surface at the single-molecule level. Our results uncover the orbital hybridization of the Au(III) center with the pi-system of the porphyrin macrocycle and visualize the size and shape of hybrid frontier orbitals in real space. In particular, the Au(III) ion contributes strongly to the highest occupied molecular orbital, which is unexpected in view of recent results and indicative of image charge effects at the molecule/substrate interface.

[1] S. Müllegger, W. Schöfberger, M. Rashidi, L. M. Reith, and R. Koch, *J. Am. Chem. Soc.* **131**, 17740 (2009).
[2] S. Müllegger, et al., *Phys. Rev. B* **83**, 165416 (2011).

(S04 – P1) Visualization of quantum dynamics of H bond within a single water dimer

Takashi Kumagai[1], Hiroshi Okuyama[2], Tetsuya Aruga[2,3], Ikutaro Hamada[4]
[1] Department of Physical Chemistry, Fritz Haber Institute of Max Planck Society, [2] Department of Chemistry, Kyoto University, Japan, [3] JST-CREST, Japan, [4] WPI-AIMR, Tohoku University, Japan

Quantum nature in H bond is important for understanding the process in wide areas of chemistry and biology, not only scientific interest. In our study, the real-space observation of the quantum dynamics for H-bond exchange has been achieved using low temperature scanning tunneling microscopy (LT-STM) [1]. By using a molecular manipulation of STM, we formed an isolated water dimer on the Cu(110) surface at 6 K with a single-molecule precision and directly observed H-bond exchange within the dimer. Time-resolved measurement of LT-STM enables us to determine the exchange rate of ~60 and ~1 Hz for H_2O and D_2O dimers, respectively, which indicates that the process is governed by quantum tunneling. In addition, theoretical calculations predicted the structure of the dimer and the reaction path (barrier) of the H-bond exchange.

[1] T. Kumagai *et al. Phys. Rev. Lett.* **100**, 166101 (2008).

(S04 – P2) Towards on-surface Bergman cyclization

Marek Kolmer[1], Szymon Godlewski[1], Jakub S. Prauzner-Bechcicki[1], Janusz Budzioch[1], Irena G. Stará[2], Ivo Starý[2], and Marek Szymonski[1]
[1] Centre for Nanometer-Scale Science and Advanced Materials, NANOSAM, Faculty of Physics, Astronomy and Applied Computer Science, Jagiellonian University, Reymonta 4, Krakow, Poland, [2] Institute of Organic Chemistry and Biochemistry AS CR, Flemingovo nám. 2, 166 10 Prague 6, Czech Republic

Large, planar, organic, aromatic, conjugated systems, like graphene, are interesting and very promising materials with respect to various future applications. However, such systems are not easily prepared, especially if one takes into account insolubility of large, planar, aromatic molecules. A possible solution of such a problem may be to deposit smaller molecules on surface from which larger molecular structures of desired properties can be manufactured. Supposedly one may use molecules that are known to undergo Bergman cyclisation process, which should generate a reactive 1,4-aryne intermediate (in the absence of hydrogen donor). Such biradical intermediates might form oligomeric structures by the recombination process. In the following presentation, preliminary ultra-high vacuum scanning tunneling microscopic (UHV-STM) experiments on two molecules capable of producing biradical intermediates through Bergman cyclisation will be discussed. Chosen molecules differ between each other only by on additional phenyl ring in defined position, both before and after cyclisation. The molecules were deposited on clean and reconstructed surface of Ge(001). Germanium is a very attractive semiconducting material from the point of view of its possible application, for instance in electronics. To obtain on-surface Bergman cyclisation two approaches were taken, either global or local. In the global approach sample with deposited molecules was first imagined with high resolution UHV-STM, thereafter annealed at elevated temperature in order to induce cyclisation process. Furthermore, it was analyzed again in search of changes that were induced in all molecules due to elevated temperature. On the other hand, in the local approach Bergman cyclisation was induced by scanning tip of the UHV-STM apparatus to a single molecule. Such an approach was possible thanks to images of single molecules obtained with very high, submolecular resolution (at room temperature). The high resolution requirement applies both to imaging before and after application of voltage pulse to a given molecule. Comparison between these two approaches for both types of molecules strongly suggests that on-surface Bergman cyclisation has been observed.

Symposium 5: **Biochemical Evolution and Protocells**

(S05 – I) Introduction

Susanna C. Manrubia

Centro de Astrobiología (INTA-CSIC). Ctra. de Ajalvir km. 4, 28850 Torrejón de Ardoz, Madrid, Spain

Life was probably ubiquitous on Earth some 3,500 million years ago. In a period that could have been as short as 100 million years, cells –very similar in structure and metabolism to extant ones— developed from abiotic matter. The pathway from inorganic chemistry to the first replicating molecule and the first functional metabolism is marked by major difficulties such as a limited availability of simple building blocks (sugars and amino acids, e.g.), a too slow rate of chemical interactions between molecules (was there a primordial pizza instead of a soup?), the formation of short homochiral polymers, an unfaithful template copy due to the low accuracy of replication, or the fragility of the initial self-sustained catalytic cycles. Stanley Miller's experiment in 1953 moved the problem of the origin of Life to the experimental sciences. Since then, significant advances have been accomplished, among them the identification of several RNA molecules able to catalyze essential chemical reactions (thus supporting the plausibility of an RNA world anterior to the current separation of functions between DNA and proteins) or the design of permeable protocells able to undergo growth and division. Experimental achievements are intimately linked to technological advances and to the development of increasingly more realistic theories addressing the different stages involved in the origin and evolution of complex chemistry and early Life.

(S05 – T1) Temperature gradient at the molecular scale: Soret effect, osmotic pressure and depletion force acting on RNA

Albert Libchaber

The Rockefeller University, 1230 York Avenue, Box #265, New York, NY 10065, USA

Results will be presented on thermophoresis of DNA and RNA. Accumulation, amplification and size sorting of DNA can be obtained in temperature gradients. We will also show how DNA and RNA can be sorted from each other and how long RNA can select short RNA. This may have implications for the origin of life hypothesis in a RNA world.

(S05 – T2) From catalytic reaction networks to protocells

Kunihiko Kaneko

Research Center for Complex Systems Biology, University of Tokyo, Japan

In spite of extensive studies to synthesize a reproducing 'protocell', there still remains a large gap between just a set of catalytic reactions and an autonomously reproducing cell. Referring also to recent experiments, I mainly discuss theoretical studies intended to fill in the gap. I will address the following questions with presenting tentative answers (or current trial-and-errors).

(S05 – T3) Reproduction of a protocell by replication of minority molecule in a mutually catalyzing cycle

Atsushi Kamimura[1], *Kunihiko Kaneko*[2]

[1] Institute of Industrial Science, The University of Tokyo, [2] Department of Basic Science, The University of Tokyo

For understanding the origin of life, it is necessary to explain the development of a compartmentalized structure, i.e., a protocell, which undergoes growth and division, from a set of chemical reactions. In this study, a hypercycle with two chemicals which mutually catalyze their replications each other is considered to show that the reproduction of a cluster of molecules with a growth-division process spontaneously happens when the replication and the degradation rates of one chemical are considerably slower than those of the other chemical, and molecules are crowded as a result of replication. It is observed that the protocell divides after a minority molecule is replicated at a slow synthesis rate, and thus, a synchrony between the reproduction of a cell and molecule replication is achieved [1]. The robustness of such protocells against the invasion of parasitic molecules is also demonstrated.

[1] A. Kamimura and K. Kaneko, Reproduction of a protocell by replication of a minority molecule in a catalytic reaction network. *Phys. Rev. Lett.*, **105**, 268103 (2010).

(S05 – P1) Plasticity, evolvability, and robustness: A macroscopic theory in terms of phenotypic fluctuations

Kunihiko Kaneko

Research Center for Complex Systems Biology, University of Tokyo, Japan

Characterization of plasticity, robustness, and evolvability is an important issue in biology. First, proportionality among evolution speed, phenotypic plasticity, and isogenic phenotypic fluctuation is derived by borrowing and extending fluctuation-response relationship in physics. Following an evolutionary stability hypothesis we derive a general proportionality relationship between the phenotypic fluctuations of epigenetic and genetic origins; the former is given by the variance of phenotype due to noise in developmental process, and the latter due to genetic mutation. The

relationship suggests a link between robustness to noise and to mutation, since robustness can be defined by the sharpness of the distribution of phenotype. Second, the proportionality between the variances is demonstrated to hold also over different phenotypic traits, when the system acquires robustness through the evolution. Third, adaptation to environmental variation is studied, which is shown to require a certain degree of phenotypic fluctuations. Indeed, the highest adaptability is achieved when the system is near the transition point to lose the robustness. Here, change in phenotypes (i.e., in the gene expression pattern) induced by environmental change is reduced later as a result of genetic evolution. All the obtained relationships are confirmed in models of gene expression dynamics, as well as in laboratory experiments. Based on our results, we revisit Waddington's canalization and genetic assimilation, and discuss how consistency between evolutionary and developmental scales constrains developmental process and leads to universal laws on phenotypic fluctuations.
K. K. *Life: An Introduction to Complex Systems Biology,* Springer (2006)**;** *PLoS One* **2**, e434 (2007), *J. Biosci.* **34**, 529 (2009); BMC Evolutionary Biology **11**, 27 (2011); Ito et al., *Mol. Sys. Biol.* **5**, 264 (2009).

Symposium 6: **Nonequilibrium Soft Matter**

(S06 – I) Introduction

Takao Ohta
Department of Physics, Kyoto University, Kyoto, 606-8502, Japan
Soft matter is a fluid having some kind of structures in a mesoscopic scale. Liquid crystals, colloids, vesicles composed of lipid molecules are typical examples. Since soft matter is easily brought into a non-equilibrium state and exhibits nonlinear response even for weak external forcing, it has attracted much attention from the view point of nonlinear science and non-equilibrium statistical physics. In this mini-symposium, we shall discuss structure and dynamics of a protein-membrane complexity, membrane dynamics of self-producing vesicles and collective dynamics of interacting self-propelled objects.

(S06 – T1) Self-reproduction of giant vesicles combined with amplification of encapsulated DNA

Tadashi Sugawara
Graduate School of Arts and Sciences, The University of Tokyo, Japan
Morphological changes of giant vesicles (GVs) usually occur associated with the change of temperature or ionic strength, etc. However we have been studying the morphological changes of GVs caused by chemical reactions. In particular, if a membrane precursor was added to a dispersion of GVs containing a catalyst, GVs grew and divided to daughter GVs with almost the same size [1]. We also reported that a robust self-reproduction of GVs continued over several generations as revealed by observation through optical microscopy and the population analysis on the basis of flow cytometric measurements [2]. As a model of a GV-based artificial cell, it is indispensible to replicate RNA/DNA in GV to deliver the information to the descendant. Hence we performed a polymerase chain reaction (PCR) using a template DNA of 1229 base-pairs (bp) and confirmed replication of the template DNA by means of a fluorescent probe (SYBR Green I) and gel electrophoresis [3]. The key point here is how to couple self-replication of DNA in GV and self-reproduction of GV. We found the GVs made of POPC, PCPG and cationic membrane molecule (V) grew and divide immediately after a membrane precursor was added to the PCR-subjected GVs (serial divisions within 15 min) [4]. Furthermore, amplified DNA was partitioned to daughter GVs. Control experiments showed that the division rate of GV without being subjected to thermal cycles of PCR was very slow (once in 2hr). The experimental results suggest that the amplified DNA adheres to the inner surface of the outer vesicular membrane and causes a budding type deformation. Besides, the formation of membrane molecule from its precursor is accelerated in the vicinity of the adhered DNA. As a result the amplification of DNA and self-reproduction of GV are linked through the chemical consequence. The appearance of self-reproducing GVs in which DNA are amplified is a milestone toward the creation of the artificial cell that gives a hint for the origin of life.
[1] K. Takakura, T. Toyota, T. Sugawara, *J. Am. Chem. Soc.,***125**, 8134, (2003); K. Takakura, T. Sugawara, *Langmuir.*, **20**, 3832 (2004); [2] T. Toyota, et al., *Langmuir* **24**, 3037-3044 (2008); K. Kurihara, et al., Soft Matter, **6**, 1888 (2010); [3] K. Shohda, et al., Soft Matter, **7**, 3750 (2011); [4] K. Kurihara, et . al., submitted for publication.

(S06 – T2) Modeling domain formation of high protein concentration at membranes of living cells

Sergio Alonso and Markus Bär
Mathematical Modelling and Data Analysis, Physikalisch-Technische Bundesanstalt, Berlin
The biochemical processes of phosphorylation and dephosphorylation are common inside of living cells. These processes consist in the reaction between kinases or phosphatases with certain proteins. The kinase adds a phosphate to the protein, consuming an ATP molecule, and the phosphatase removes the phosphate from the protein. The introduction of the phosphate changes the electrical properties of the proteins. Here we consider that the free proteins tend to bind at the membranes and the complex protein/phosphate unbinds from the membrane. Due to the difference on the diffusion coefficients of the proteins at the membrane and on the cytoplasm the asymmetry on the phospharylation

and the dephosphorylation may produce the domain formation of high protein concentration at the membrane. We apply this study to the particular case of MARCKS proteins in vivo [1] and in vitro [2].
[1] S. Alonso and M. Bär. Phase separation and bistability in a three-dimensional model for protein domain formation at biomembranes, *Phys. Biol.* **7**, 0460112 (2010).
[2] S. Alonso, U. Dietrich, C. Händel, J. A. Käss and M. Bär. Oscillations in the lateral pressure of lipid monolayers induced by nonlinear chemical dynamics of the second messengers MARCKS and Protein kinase C. *Biophys. J.* **100**, 939947 (2011).

(S06 – T3) Alignment vs. noise: Minimal models for collective motion

Hugues Chaté
Service de Physique de l'Etat Condensé, CEA Saclay, F-91191 Gif-sur-Yvette, France

(S06 – T4) Hydrodynamic interactions in populations of simple model squirmers with tunable velocites

Shashi Thutupalli[1], *Ralf Seemann*[1,2], *Stephan Herminghaus*[1]
[1] Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany, [2] Physics Department, University of Saarland, Saarbrücken, Germany

We present a scheme of self-propelling liquid droplets which closely mimics the locomotion of some protozoal organisms, so-called squirmers. In contrast to other schemes proposed earlier, locomotion paths are not self-avoiding, since the effect of the squirmer on the surrounding medium is weak. Our results suggest that not only the velocity, but also the mode of operation (i.e., the spherical harmonics of the flow field) can be controlled by appropriate variation of parameters. The model squirmers are experimentally realized using monodisperse aqueous droplets containing chemicals that produce a steady source of bromine ions, in an external oil phase rich in surfactant. The surfactant (mono-olein) reacts at the droplet interface with the bromine produced within the droplets, and a dynamic instability leads to gradients of interfacial tension at the droplet interface. These gradients set up Marangoni stresses at the droplet interface, thus propelling the droplets. The motion mechanism closely resembles that of a squirmer due to the surface tangential velocities at the droplet interface. The flow around the swimmers as well as its effect on the droplet motion are measured using particle image velocimetry (PIV). The PIV analysis reveals the far field flows generated by the swimmers in the surrounding liquid, leading to the emergence of bound states and oriented clusters.
[1] S. Thutupalli, R. Seemann, S. Herminghaus, *Simple model squirmers with tunable velocity*, submitted (2011).

(S06 – P1) Shape transitions of self-propelled droplets induced by Korteweg force

Takahiko Ban[1], *Tomohiro Yamada*[2],
[1] Department of Materials Engineering Science, Graduate School of Engineering Science, Osaka University, [2] Department of Chemical Engineering & Materials Science, Doshisha University

We experimentally show the self-generated motion and deformation of phase-separating droplets using an aqueous two-phase system. The motion and deformation depends on the composition of the continuous phase [1]. The behavior is due to the coupling between mass and momentum transfer via Korteweg force which arises from minimizing the free energy of the system and is proportional to the chemical potential gradient [2]. Differently from the numerical simulation by Vladimirova et al, the droplets moved unidirectionally and showed the shape transitions. In the study, we investigated the cause by measuring of flow pattern and concentration profile inside and outside the droplets.
[1] T. Ban, A. Aoyama, and T. Matsumoto, *Chem. Lett.*, **39**, 1294 (2010).
[2] D. J. Korteweg, *Arch. Néerl. Sci. Exactes Nat.*, **6**, 1 (1901).
[3] N. Vladimirova, A. Malagoli, and R. Mauri, *Phys. Rev. E* **60**, 2037 (1999).

(S06 – P2) Molecular machines in biomembranes: A mesoscopic model study including the solvent effects

Mu-Jie Huang[1], *Raymond Kapral*[2], *Alexander Mikhailov*[3], *Hsuan-Yi Chen*[1]
[1]Department of Physics and Institute of Biophysics, National Central University, Jhongli 32001, Taiwan, [2]Chemical Physics Theory Group, Department of Chemistry, University of Toronto, Ontario, Canada, [3]Abteilung Physikalische Chemie, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany.

Coarse-grained descriptions are used to model operation of molecular machines in lipid bilayers in the presence of solvent. Elastic-network model for a molecular machine in a dense environment described by multiparitcle collision dynamics [1] is combined with a coarse-grained model [2] for biomembranes. By using the resulting mesoscopic model, operation cycles of a membrane molecular machine could be simulated including the hydrodynamical effects. Effects of active protein inclusions on the memrane dynamics are thus considered.
[1] A. Cressman, Y. Togashi, A. S. Mikhailov, and R. Kapral, *Phys. Rev. E* **77**, 050901 (2008).
[2] I. R. Cooke, K. Kremer, and M. Deserno, *Phys. Rev. E* **72**, 011506 (2005).

(S06 – P3) Motion of a cm-sized oil droplet on water surface driven by light

Masatoshi Ichikawa[1], *Takafumi Iwaki*[2], *Keitaro Miura*[1], *Nobuyuki Magome*[3], *Kenichi Yoshikawa*[1]
[1] Department of Physics, Graduate School of Science, Kyoto University, [2] Fukui Institute for Fundamental Chemistry, Kyoto University,[3] Institute for Integrated Cell-Material Sciences (iCeMS), Kyoto University, Japan

Locomotor activity of the oil droplet is studied. Liquid paraffin droplet put on the aqueous phase was vertically irradiated with laser light. Since the laser light with 532 nm in wavelength is absorbed efficiently in a red dye dissolved in the oil droplet, temperature distribution was generated inside the droplet. Light itself does not act directly on the motion of the oil droplet, therefore, the present experiment sets up a self-propelling droplet driven by a non-contact temperature field inside the oil droplet. Locally irradiated laser induces internal and external convection of the fluids, and the droplet moves. Driving force of this movement is considered to be mainly due to Marangoni flow which is produced by interfacial tension gradient on the oil/water interface. Motion and dancing of the droplet is discussed with our previous study [1].

[1] S. Rybalko, N. Magome, K. Yoshikawa, *Phys. Rev. E* **70**, 046301 (2004).

(S06 – P4) Nonlinear flow behavior in mixing and reaction processes between a water-soluble polymer solution and a metal ion

Yuichiro Nagatsu[1], *Asami Nagae*[1], *Mitsumasa Ban*[1], *Shuichi Iwata*[1], *Yutaka Tada*[1]
[1] Department of Materials Science and Engineering, Graduate School of Engineering, Nagoya Institute of Technology, Gokiso-cho, Showa-ku, Nagoya, Aichi, 466-8555, Japan

We have experimentally investigated mixing and reaction processes between a partially hydrolyzed polyacrylamide (PAM) solution and ferric ion. We added a solution including ferric ion to a vessel in which the PAM solution was stirred by an impeller at a constant rotational speed. We observed flow behavior in the vessel during and after the addition of the ferric ion solution. We found nonlinear flow behavior. After the addition of the ferric ion solution, Weissenberg effect started to occur. It should be noted that Weissenberg effect is not observed before the addition in the present experimental condition. When the rotation of the impeller was kept, Wessenberg effect gradually disappeared and a free surface of the solution finally became flat. In order to elucidate mechanism for the observed transient phenomenon, some measurements by means of a rheometer have been performed. Finally, we propose the mechanism associated with interaction between ferric ion and the polymer chain.

(S06 – P5) Spontaneous mode switching of a self-running solid/liquid composite

Fumi Takabatake[1], *Nobuyuki Magome*[2], *Masatoshi Ichikawa*[1], *Kenichi Yoshikawa*[1]
[1] Department of Physics, Graduate School of Science, Kyoto University
[2] Institute for Integrated Cell-Material Sciences (iCeMS), Kyoto University, Japan

Recently, spontaneous motions of liquid droplets, solid particles and gels under non-equilibrium conditions have been actively studied [1]. In the present paper, we report [2] that a solid/liquid composite exhibits regular spontaneous motions under isotropic boundary conditions, driven by chemical Marangoni effect. When an oil droplet of oleic acid merged with a solid sodium oleate is placed on a water phase, the composite undergoes specific spontaneous motion, such as translational, spinning, or orbital motion, depending on the relative size of the solid sodium oleate with respect to that of the oil droplet. The essential features of such mode-switching are reproduced by using ordinary differential equations by taking into account of the spontaneous symmetry breaking under a dissipative condition.

[1] J. Tersoff, D. E. Jesson, W. X. Tang, *Science*, **324**, 236 (2009).
[2] F. Takabatake, N. Magome, M. Ichikawa, K. Yoshikawa, *J. Chem. Phys.*, **134**, 114704 (2011).

Symposium 7: **Electrochemistry and Surface Reactions**

(S07 – I) Introduction

K. Krischer
Department of Physics, Technical University of München, Germany

(S07 – T1) Dynamics of electrochemical CO oxidation in PEM fuel cells

Kai Sundmacher[1,2], *Richard Hanke-Rauschenbach*[1], *Sebastian Kirsch*[1], *Liisa Rihko-Struckmann*[1]
[1] Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg, [2] Process Systems Engineering, Otto-von-Guericke University Magdeburg

The operation of polymer electrolyte membrane (PEM) fuel cells with reformate gas mixtures requires the reduction of the CO feed gas content down to a level of 10 ppm. For this purpose, Zhang et al. [1] have proposed an electrochemical preferential oxidation (ECPrOx) reactor designed similarly as a PEM fuel cell. In the present contribution, the dynamic operational behavior of this ECPrOx reactor is analyzed based on experimental data and mathematical models. First, the influence of the feed flow rate and CO-content on the behavior of a well-mixed ECProX unit is discussed [2]. Then, the role of concentration and potential distributions on the formation of spatial-temporal patterns in a distributed ECPrOx reactor is investigated [3].

[1] J.X. Zhang, R. Datta. *J. Electrochem. Soc.*, **152**, A1180 (2005).
[2] R. Hanke-Rauschenbach, C. Weinzierl, M. Krasnik, L. Rihko-Struckmann, H.Lu, K. Sundmacher. *J. Electrochem. Soc.,* **156**, B1267 (2009).

[3] R. Hanke-Rauschenbach, S. Kirsch, R. Kelling, C. Weinzierl, K. Sundmacher, *J. Electrochem. Soc.*, **157**, B1521 (2010).

(S07 – T2) Geometry-dependent universal fluctuations of growing interfaces: evidence in turbulent liquid crystals

Kazumasa A. Takeuchi[1,2], *Masaki Sano*[1]
[1] Department of Physics, the University of Tokyo, Japan,[2] SPEC, CEA-Saclay, France

To what extent can scale-invariant phenomena be universal in systems driven out of equilibrium? As an answer to this question, we present our experimental results on interface growth of electrically-driven turbulent liquid crystals, which turns out to show unprecedented universality beyond the mere scaling laws: Growing interfaces of topological-defect turbulence exhibit not only the universal scaling laws of the Kardar-Parisi-Zhang class, which is the basic class for stochastic surface growth problems, but even universality in the distribution and correlation functions for the interface fluctuations. The distribution agrees quantitatively with the one studied in the completely different context of random matrix theory – namely the largest-eigenvalue distribution of Gaussian random matrices – and depends on whether the growing interfaces are curved or flat on average, albeit universal in each case. This provides a strong experimental evidence for the universality underlying scale-invariant growth processes driven out of equilibrium.

[1] K. A. Takeuchi and M. Sano, *Phys. Rev. Lett.* **104**, 230601 (2010) and forthcoming papers.

(S07 – T3) Experimental observation of the effect of a low coupling strength on pattern formation during HCOOH electro-oxidation on a Pt ring electrode

Adriana Bernal-Osorio, Markus Eiswirth
Dept. of Physical Chemistry, Fritz-Haber-Institut der Max-Plank Gesellschaft, Berlin

The dependence of the coupling effect on the conductivity of the electrolyte, and its effect on the occurrence of travelling patterns has been studied during the electro-catalytic oxidation of formic acid (HCOOH) on platinum (Pt). At lower conductivities, when the coupling trough the electrode is weak, localized patterns, i.e. localized bursts, are present, followed by standing waves. On the other hand, travelling patterns like rotating pulses are favored over the occurrence of localized oscillations at higher conductivities. All experiments were carried out at potentiostatic conditions.

(S07 – T4) *In-situ* visualization of pitting corrosion on stainless steel

Peter E. Klages, Harm H. Rotermund
Dept. of Physics and Atmospheric Science, Dalhousie University, Halifax, NS, Canada

While stainless steels and aluminum alloys are designed to resist corrosion, they are still susceptible to localized corrosion, which can lead to failure and the possibility of catastrophic events as a result. To study the beginning steps of one type of localized corrosion, pitting corrosion, different *in-situ* visualization techniques for the stainless steel-electrolyte were developed, including the simultaneous use of contrast-enhanced microscopy and EMSI (ellipsometric microscopy for surface imaging). These methods have helped in explaining the sudden onset of corrosion as an explosive autocatalytic growth in number of metastable pits [1], and have given evidence for the weakening of the oxide layer and front movement as a component of the pitting corrosion process, consistent with stochastic reaction-diffusion systems [2]. Recent work has added a third simultaneous *in-situ* visualization technique, digital in-line holographic microscopy, for the investigation of the electrolyte in close proximity to the stainless steel sample being studied. This method is being used to track ejected material from long-lived pits through a small volume of the electrolyte, as well as to help locate metastable pitting events as small as 100 nA. The scale of metastable pits detected is dependent on the sample position with respect to the point light source, but the fact that events are still observable even in more extreme orientations gives evidence for local changes in the electrolyte itself during an event.

[1] C. Punckt, et al., Sudden onset of pitting corrosion as a critical phenomenon. *Science,* **305**, 1133-1136 (2004).
[2] M. Dornhege, et al., Spreading of corrosion on stainless steel, *J. Electrochem. Soc.,* **154**, C24-C27 (2007).

(S07 – P1) Pattern formation in CO electrooxidation

Philipp Bauer
Physik-Department, Technische Universität München, Garching

(S07 – P2) Entrainment in a forced spatially extended electrochemical system with negative global coupling

Tahmineh Pourrostami[1], *Adrian Birzu*[2], *Katharina Krischer*[1]
[1] Physik-Department, Technische Universität München, Garching, [2] Faculty of Chemistry, Al. I. Cuza University, Iasi, Romania

We present experiments of an externally forced electrochemical oscillator with an intrinsic negative global coupling. The electrochemical system studied is the oxidation of H_2 on a Pt ring electrode in the presence of Cu^{2+} and Cl^- ions. An external negative impedance gives rise to a global coupling that destabilizes the uniform relaxation oscillations. At certain parameter values it induces stable pulses, which constitute our reference state [1]. The forcing is realized by adding a sinusoidal variation on the externally applied voltage. We studied the response of the pulses as a function of amplitude and frequency of forcing. It differs significantly from the one reported for oscillatory media without global

coupling. Within the entire frequency range up to large amplitudes the dynamics exhibits nontrivial patterns. Only at the largest forcing amplitudes used were uniform oscillations stable. In the 1:1 tongue, a low forcing amplitude lead to the entrainment of the *local oscillators;* thus the pulse solution were stabilized while the global signals stayed stationary. At higher forcing amplitudes the pulses develop a defect line and the entrainment affects the uniform mode in addition. When further increasing the forcing amplitude, more complicated locking patterns established. Within the 2:1 resonance tongue, which is the broadest, 2-phase cluster patterns prevailed. When crossing the tongue, we observed standing as well as traveling 2-phase clusters, pointing to the existence of an Ising-Bloch bifurcation. In the superharmonic region, the entrainment tends to enhance modulation of the pulse width.

[1] P. Grauel, H. Varela, K. Krischer, Spatial bifurcations of fixed points and limit cycles during the electrochemical oxidation of H_2 on Pt ring-electrodes, *Faraday Discussions*, **120**, 165 (2001).

(S07 – P3) Large improvement of efficiency under erratic galvanostatic time pattern in PEMFCs

Andressa Mota[1,2 *] *Ernesto R. Gonzalez*[2], *Markus Eiswirth*[1,3]

[1] Dept. of Physical Chemistry, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany, [2] IQSC- USP, Av. Trab. Sancarlense 400, CEP 13560-970. São Carlos-SP, Brazil, [3] Ertl Center for Electrochemistry and Catalysis, GIST, Cheomdan-gwagiro 261, Buk-gu, Gwangju 500-712, South Korea

This work aims to provide empiric evidence on how Polymer Electrolyte Membrane (PEM) fuel cells (FCs) in different oscillatory states could show improvement of the efficiency compared to a poisoned monotonic stationary state. The discussion is based on the analytic analysis of the irreversible dissipation equation. The experimental results suggest that an erratic oscillatory time pattern largely improves the efficiency compared to the simplest time pattern as time series with only one period (p1).

(S07 – P4) Model-based identification of a spatial bifurcation in the electro-oxidation of H_2-CO mixtures on Pt

Elizeth Ramírez-Álvarez[1], *Katharina Krischer*[2], *Ramiro Rico-Martínez*[1]

[1] Department of Chemical Engineering, Instituto Tecnológico de Celaya, México, [2] Department of Physics, Technical University of München, Germany

In this contribution, a previously developed strategy for identification of a nonlinear model from spatio-temporal experimental observations [1] is extended for real-time detection of bifurcations. The identified model is used as reference for tracking the dynamic evolution of the system; allowing the compensation of modeling errors, noise and drift in real-time via a modified Kalman filter [2]. The application for the detection of a spatial bifurcation observed during the electro-oxidation of H_2-CO mixtures on platinum under galvanostatic conditions is described, based on the protocol for bifurcation detections proposed in [3].

[1] K. Krischer, R. Rico-Martínez, I.G. Kevrekidis, H.H. Rotermund, G. Ertl and J.L. Hudson. Model Identification of spatiotemporally varying catalytic reaction. AIChE *J.*, **39**, 89-98 (1993).

[2] Ramírez-Álvarez E., Rico-Martínez R. and Parmananda P., Chaos induction using a reference model assisted control. *J. Phys, Chem.,* **114** (49), 12819–12824 (2010).

[3] R. Rico-Martínez, K. Krischer, G. Flätgen, J. S. Anderson and I.G. Kevrekidis. Adaptive detections of instabilities: an experimental feasibility study. *Physica D*, **176**, 1-18. (2003).

Symposium 8: **Control of Self-Organization Processes**

(S08 – I) Introduction

E. Schöll

Institute for Theoretical Physics, Technical University of Berlin, Germany

(S08 – T1) Spatially forced thermal convection

Gabriel Seiden[1], *Stephan Weiss*[2], *Eberhard Bodenschatz*[3]

[1] Department of Physics of Complex Systems, Weizmann Institute of Science, Rehovot, Israel,[2] Department of Physics, UCSB,3 Department of Hydrodynamics, Pattern Formation and Nanocomplexity, Max Planck Institute for Dynamics and Self-Organization, Goettingen

Spatial forcing of pattern forming systems is a valuable tool in investigating stability regions in parameter space and the emergence of novel patterns, as well as in studying suppression and control of spatiotemporal chaos. Here we report experiments on spatially forced inclined layer convection, where the combined effect of the intrinsic symmetry breaking due to a gravity-induced shear flow and a spatially periodic 1D forcing in the form of surface corrugations is studied. We observed pattern selection processes resulting in stabilization of spatiotemporal chaos and the emergence of novel two-dimensional states.

(S08 – T2) Feedback control of 2D wave segments in cortical excitable media

Markus A. Dahlem *and Eckehard Schöll*
Institute for Theoretical Physics, Technical University of Berlin, Germany

A mechanism is presented by which a traveling excitation wave causing migraine is formed in the 2D folded human cortex. The predicted cortical wave assumes a characteristic form (shape, size, and duration) on a curved surface that also has been observed in a clinical study using functional magnetic resonance imaging. Using our understanding of dynamics in terms of phase space trajectories, we develop feedback control concepts, which might eventually allow for suppressing these excitation waves and thus treating dynamical disease. We propose that migraine is such a dynamical disease and we explore new ways to develop therapeutic strategies, in particular, time-delayed feedback control that can be used to intelligently target migraine.

(S08 – T3) Taming electrical turbulence in the heart

Stefan Luther[1,2,3]
[1] Max Planck Institute for Dynamics and Self-Organization, Goettingen, Germany,[2] Institute for Nonlinear Dynamics, Georg August Universitaet, Goettingen, Germany,[3] Department of Biomedical Sciences, Cornell University, Ithaca, NY, USA

The control of defect turbulence, as manifested by catalytic surface reactions, spiral-defect-chaos, or cardiac excitations, remains a scientific challenge. For lack of a better strategy, strong, globally resetting electrical shocks are employed to control cardiac fibrillation – a life-threatening electric defect turbulent state. We show that concepts from nonlinear physics suggest an alternative. We find that a weak electric pulse triggers wave emission from discontinuities in electrical conductivity of the cardiac tissue, that the number of wave-emitting sites can be tuned with the applied field, and that the three-dimensional electric turbulence is controllable by pacing at low pulse energies [1,2]. Using optical mapping in isolated perfused canine atrial preparations, we show that a series of pulses at low field strength (0.9 to 1.4 V/cm) is sufficient to entrain and subsequently extinguish atrial fibrillation with a success rate of 93% (69 of 74 trials in 8 preparations), using only 13% of the energy per pulse required by a single shock ($P < 0.002$). Our results not only provide an experimental proof of far-field control of electrical turbulence in the heart, but also open new research perspectives towards alternative, life-saving defibrillation techniques.

[1] F.H. Fenton et al., Termination of Atrial Fibrillation Using Pulsed Low-Energy Far-Field Stimulation, *Circulation,* **120,** 467-476 (2009).
[2] A. Pumir et al., Wave Emission from Heterogeneities Opens a Way to Controlling Chaos in the Heart, *Phys. Rev. Lett.,* **99**, 208101 (2007).

(S08 – T4) Destabilization of localized structures in reaction-diffusion systems induced by delayed feedback

Svetlana Gurevich *and Rudolf Friedrich*
Institute for Theoretical Physics, University of Münster, Germany

We are interested in the stability of one- and two-dimensional localized structures in reaction-diffusion systems subjected to a delayed feedback. We investigate the spectral properties of the delayed system and show that the presence of the delayed feedback term can induce complex behavior of the localized structures, including, e.g., spontaneous motion and breathing of the localized objects. In the case of spontaneous motion, corresponding order parameter equations for the position of the localized structure is derived. In addition, numerical simulations are carried out showing good agreement with the analytical predictions.

(S08 – T5) Synchronization of Dissipative Optical Solitons

D. Laroze[1,2], *J. Bragard*[3], *J. Elorza*[3], *P. Diaz*[4], *H. Pleiner*[1], *O. Descalzi*[5]
[1] Max Planck Institute for Polymer Research, Mainz, Germany, [2] Instituto de Alta Investigacion, Universidad de Tarapaca, Arica, Chile, [3] Departamento de Fisica y Matematica Aplicada, Universidad de Navarra, Spain, [4] Departamento de Fisica, Universidad de la Frontera, Temuco, Chile,[5] Facultad de Ingenieria, Universidad de los Andes, Santiago, Chile

We study the synchronization between different moving localized structures in an optical system. We use as prototype model a set of two coupled cubic quintic complex Ginzburg-Landau equations. Such a model accepting stable localized structures as solutions has a direct physical interpretation, e.g. for a dual-core fiber laser. The interaction between the fields is chosen to be linear because this type of coupling is used to model ring lasers based on dual-core fibers [1]. Starting with different initial states, one can have a simple stationary dissipative soliton or a breathing pulse. Both fields become synchronized after a transient. Finally, we remark that the type of synchronization [2] strongly depends on the specific form of the coupling between the fields.

[1] K. Porsezian, R. Murali, B. A. Malomed, R. Ganapathy, *Chaos, Solitons and Fractals* **40**, 1907 (2009).
[2] S. Boccaletti, J. Kurths, G. Osipov, D.L. Valladares, C.S. Zhou, *Physics Reports* **366,** 1 (2002).

(S08 – P1) Giant subharmonic Arnold' tongues in a system of globally coupled FitzHugh-Nagumo oscillators with time-periodic coupling strength

Adrian Bîrzu[1,2], *Katharina Krischer*[2]
[1] Faculty of Chemistry, Al. I. Cuza University of Iaşi, Romania, [2] Physik Department E19a, Technische Universität

München, Garching

We investigate numerically the dynamics of a population of globally coupled FitzHugh–Nagumo oscillators with a time-periodic coupling strength. While for synchronizing global coupling, the in-phase state is always stable, the oscillators split into several cluster states for desynchronizing global coupling, most commonly in two, irrespective of the coupling strength. The prevalence of two and four cluster states leads to large 2:1 and 4:1 subharmonic resonance regions, while at low coupling strength for a harmonic 1:1 or a superharmonic 1:m time-periodic coupling coefficient, any resonances are absent and the system exhibits nonresonant phase drifting cluster states. Furthermore, in the unforced, globally coupled system the frequency of the oscillators in a cluster state is in general lower than that of the uncoupled oscillator and strongly depends on the coupling strength. Periodic variation of the coupling strength at twice the natural frequency causes each oscillator to keep oscillating with its autonomous oscillation period. The behavior of the FitzHugh-Nagumo oscillators is compared to two systems of globally coupled electrochemical oscillators of N-NDR and HN-NDR type, respectively.

[1] A. Bîrzu, K. Krischer. Resonance tongues in a system of globally coupled FitzHugh-Nagumo oscillators with time-periodic coupling strength, *Chaos*, **20**, 043114 (2010).

(S08 – P2) Homopolymers effects in BZ-AOT system under Turing conditions

Jorge Carballido-Landeira[1]*, Alberto P. Muñuzuri*[1]
[1] Group of Nonlinear Physics, University of Santiago de Compostela, Spain

Water-in-oil microemulsion loaded with a reaction-diffusion chemical system (Belousov-Zhabotinsky reaction) is able to exhibit Turing patterns [1] that are believed to be responsible for differentiation processes in Nature. Using polymers, as polyethylene oxide, longer than the droplet size we are able to change the distribution of droplets due to cluster formation [2]. This difference in the nanoscale has relevant consequences in the observed Turing pattern's wavelength, which is three orders of magnitude larger than the droplet size [3].

[1] I. R. Epstein and V. Vanag, *Chaos*, **15**, 047510 (2005).
[2] C. Laia W. Brown, M. Almgren and S. M. B. Costa, *Langmuir*, **16**, 465–470 (2000).
[3] J. Carballido-Landeira, P. Taboada and A. P. Muñuzuri, *Phys. Chem. Chem. Phys.,* **13**, 4596-4599 (2011).

(S08 – P3) Pattern formation in the iodate-sulfite-thiosulfate reaction-diffusion system

Haimiao Liu[1]*, Lin Ren*[1]*, John A. Pojman*[2]*, Qingyu Gao*[1]
[1] College of Chemical Engineering, China University of Mining and Technology, [2] Department of Chemistry, Louisiana State University

As ideal model system and a powerful tool for understanding biological development, pattern formation in solution chemistry has been a paradigm and a leading area [1,2]. Over the past two decades, spatiotemporal pattern formation in chemical reaction-diffusion systems has achieved remarkable developments since the first experimental discovery of Turing patterns in the chlorite-iodide-malonic acid (CIMA) system in 1990 [3]. Sustained spiral waves mainly focus on the classical Belousov-Zhabotinsky (BZ) reaction. Spatial stationary patterns such as Turing patterns mostly centered on the CIMA reaction, the Belousov-Zhabotinsky in aerosol OT microemulsion (BZ-AOT) system [4]. And a large variety of spatial patterns such as stationary labyrinthine patterns, self-replicating spots arising from front interactions and front instabilities were observed in the ferrocyanide-iodate-sulfite (FIS) reaction [5]. In recent ten years, De Kepper's group was dedicated to design different pattern formation ranging from spatial bistability, spatial oscillations to Turing patterns [6]. For the analogous Landolt-type iodate-sulfite-thiosulfate (IST) reaction, which is autocatalytic for both protons and iodide ions, shows complex oscillations in a continuously flow stirred tank reactor (CSTR) [7] and produces pH waves and iodine waves in a petri dish [8]. We investigated the starch-induced iodine pattern formation and the sodium polyacrylate induced pH pattern formation in the IST reaction in a one-side fed disc gel reactor. As binding agents of the autocatalyst of hydrogen ion or iodide ion, different content of sodium polyacrylate or starch has selectivity on the pattern formation. We observed the iodine pulses, branched patterns, and labyrinthine patterns occurred upon increasing the starch content in the system, and observed the pH pulses, striped patterns, mixed spots and strips, and hexagonal spots upon increasing the content of sodium polyacrylate. Coexistence of pH fronts and iodine fronts was also studied in a batch IST reaction-diffusion system. The phenomenon of both pH and iodine wave instability such as cell fronts and Turing structure were observed in the presence of sodium polyacrylate by perturbations.

[1] R. Kapral, K. Showalter, Eds. *Chemical Patterns and Waves* (Kluwer Academic Publisher, Amsterdam, The Netherlands, 1995).
[2] I. R. Epstein, J. A. Pojman, *An Introduction to Nonlinear Chemical Dynamics* (Oxford University Press, New York, America, 1998).
[3] V. Castets *et al.*, *Phys. Rev. Lett.*, **24**, 2953 (1990).
[4] V. K. Vanag, I. R. Epstein, Chapter 5. In *Patterns of Nanodroplets: The Belousov-Zhabotinsky-Aerosol OT-Microemulsion System* (Springer, Berlin, 2008).
[5] K. J. Lee *et al.*, *Science*, **261**, 192 (1993).
[6] J. Horváth, I. Szalai, P. De Kepper, *Science*, **324**, 772 (2009).
[7] H. Liu, J. Xie, L. Yuan, Q. Gao, *J. Phys. Chem. A,* **113**, 11295 (2009).
[8] Q. Gao, R. Xie, *Chem. Phys. Chem,* **9**, 1153 (2008).

(S08 – P4) Control of activation sites by low-electric far field pacing

Marcel Hörning[1], Seiji Takagi[2], Kenichi Yoshikawa[1]
[1] Dept. of Physics, Graduate School of Science, Kyoto University, Kyoto, Japan
[2] Research Institute for Electronic Science, Hokkaido University, Sapporo, Japan

Termination of cardiac arrhythmias and fibrillation in the beating heart is currently treated with antitachycardia pacing or cardioversion. However, those have its drawbacks, either having a restricted application or producing undesirable side effects. The method of low-energy far field stimulation is an improved therapy introduced recently, suggesting that the application of low electric far field shocks can induce a large number of activation sites ("virtual electrodes") in the tissue that permits to terminate undesired states in heart [1]. In this study we investigate in the activation site density depending on the applied electric field in in-vitro experiments of cardiac tissue culture. It was found that the activation site density increases exponentially depending on intracellular conductivity and the level of cell isotropy. Additionally, we reproduce quantitatively the experimental results by numerical bidomain simulations and derive an intuitive framework that describes the activation site density with that we are able to determine the ratio of longitudinal and transverse conductivity to 2.8 in in-vitro experiments of cardiac tissue culture.

[1] F. Fenton et al., Termination of Atrial Fibrillation Using Pulsed Low-Energy Far-Field Stimulation. *Circulation,* **120**, 467 (2009).

(S08 – P5) Control of Turing patterns and their usage as logic gates and sensors

František Muzika, Igor Schreiber
Department of Chemical Engineering, Institute of Chemical Technology, Prague, Center for Nonlinear Dynamics of Chemical and Biological Systems, Technická 5, 166 28, Praha 6, Czech Republic

We focus on finding parameters for occurrence of Turing patterns (spatially nonuniform steady states) in the model of three coupled ideally mixed continuous stirred tank reactors arranged in a linear array. In the context of interacting cells (or subcellular units) in organisms, we took a two-variable core model of glycolysis due to Moran and Goldbeter occurring within each unit that interacts by diffusive transport with adjacent units. First, we identify Turing patterns in the system at various inhibitor-activator ratios of transport coefficients by constructing solution diagrams with a free parameter being the inhibition rate coefficient. In particular, we chose the inhibitor/activator ratios 100/1, 1/1 and 4/5. Stable Turing patterns occur in all three cases. However, spontaneous transition from a stable spatially uniform steady state to a Turing pattern occurs only in the first case, while the other two cases possess Turing patterns stabilized by secondary bifurcations that coexist with uniform periodic oscillations. Next, we found series of modular spatiotemporal perturbations, which allow for accessing Turing patterns from the oscillatory mode in the case with the inhibitor-activator ratio equal one. Applying such perturbations to the system with coexisting stable uniform oscillations and three distinct types of Turing patterns allows us to control, which Turing pattern and/or oscillation will occur. Since the occurrence of Turing patterns can be controlled, we propose the system to function as: 1) a sensor capable of reading certain value of concentration, 2) a memory array capable of storing information digitally, 3) three-input logic gates XOR+AND and NAND+OR.

(S08 – P6) Phase description of nonlinear dissipative waves under space-time-dependent external forcing

Yousuke Tonosaki[1], Takao Ohta[1], Vladimir Zykov[2]
[1] Department of Physics, Kyoto University,[2] Institut fuer Theoretische Physik, Technische Universitaet Berlin

Based on the model system undergoing phase separation and chemical reactions, we investigate the dynamics of propagating dissipative waves under external forcing which is periodic both in space and time. A phase diagram for the entrained and non-entrained states under the external forcing is obtained numerically. Theoretical analysis in terms of phase description of the traveling waves is carried out to show that the transition between the entrained and the non-entrained states by changing the external frequency occurs either through a saddle-node bifurcation or through a Hopf bifurcation and that these two bifurcation lines are connected at a Bogdanov-Takens bifurcation point. The phase equations of motion given by theoretical analysis also have a propagation reversal solution. This solution comes from that the original system has two solutions propagating to the right and the left equivalently by isotropy of space.

Symposium 9: **Active Particles**

(S09 – I) Introduction

L. Schimansky-Geier
Dept. of Physics, Humboldt University of Berlin, Germany

(S09 – T1) Collective dynamics of microswimmers

Ayusman Sen
Department of Chemistry, The Pennsylvania State University, University Park, PA 16802, USA

One of the more interesting recent discoveries has been the ability to design nano/microparticles, which catalytically harness the chemical energy in their environment to move autonomously. These "bots" can be directed by chemical and light gradients. Further, our group has developed systems in which chemical secretions from the translating micro/nanomotors initiate long-range, collective interactions among the particles via self-diffusiophoresis. This behavior is reminiscent of quorum sensing organisms that swarm in response to a minimum threshold concentration of a signaling chemical. We will discuss recent experimental results, as well as approaches to the modeling of the complex emergent behavior of these particles.

(S09 – T2) Motion analysis of self-propelled Pt-Silica particles in hydrogen peroxide solutions

H. Ke[1]*, S. Ye*[1]*, R. L. Carroll*[1]*, K. Showalter*[1]
[1]C. Eugene Bennett Department of Chemistry, West Virginia University, Morgantown, WV, USA

Silica microspheres that are half coated with platinum metal undergo self-propulsion in solutions of H_2O_2, with the average speed increasing with increasing H_2O_2 concentration. Microscopic observation of the particle motion, with segmentation of the image data, demonstrates that the particles move, on average, with the platinum coated region oriented opposite to the direction of motion. Velocity autocorrelation and motion direction analyses show that the direction of motion is highly correlated with the particle orientation. The effect of the observation time interval on the measured translational diffusion coefficient and the apparent particle motion is analyzed.

[1] H. Ke, S. Ye, R. L. Carroll, K. Showalter. Motion analysis of self-propelled Pt-Silica particles in hydrogen peroxide solutions, *J. Phys. Chem. A*, **114**, 5462 (2010).

(S09 – T3) Ratcheted colloids: From single particle enhanced diffusion to Rouse-like collective behavior

Francesc Sagués, Pietro Tierno
Physical Chemistry Department, University of Barcelona, Spain

Transport and diffusion in periodic and random potentials play a key role in many different contexts of Physics, Chemistry and Biology. Here we report recent experimental results related to the transport mode of paramagnetic particles dispersed on a uniaxial garnet film, which exhibit a longitudinal ratchet effect in the presence of an oscillating magnetic field.

First we concentrate on the transversal wandering of single particles. As compared to situations free from magnetic forcing, this motion is characterized by a giant enhancement of the diffusion coefficient by almost four decades and a pronounced maximum depending on the driving frequency. This behavior is rationalized in terms of a model that takes into account the presence of a random transversal disorder periodically refreshed as the particle is transported above the film [1]. The second considered scenario refers to the collective behavior of a chain of these particles. The center of mass of the chain shows a diffusive behavior, while its end-to-end distance displays anomalous subdiffusive growth. We interpret the experimental data by using the Rouse model, originally developed for polymers, and extract the potential of mean-force and all relevant parameters [2].

[1] P. Tierno, P. Reimann, T. H. Johansen, F. Sagués. Giant transversal particle diffusion in a longitudinal magnetic ratchet, *Phys. Rev. Lett.*, **105**, 230602 (2010).
[2] P. Tierno, F. Sagués, T. H. Johansen, I. M. Sokolov, (submitted to *Soft Matter*).

(S09 – P4) Polar order in active colloidal suspensions

Mihaela Enculescu, Holger Stark
Institute for Theoretical Physics, Technical University of Berlin

We consider theoretically the sedimentation of a dilute suspension of chemically powered colloids, so-called active Brownian particles. This system has been studied experimentally and it was found that the sedimentation length increases with the propulsion velocity of the particles [1]. We derive a Smoluchowski equation for non-interacting active Brownian particles subject to gravity as well as translational and rotational diffusion. We determine the steady sedimentation profile of the suspension both by perturbation analysis and by numerically solving the Smoluchowsky equation. We show that sedimentation is accompanied by polar order of the active particles, with the mean swimming velocity oriented against the gravitational field. We suggest realistic parameter values to observe this ordering which increases strongly with the particle radius. The origin of the predicted polar order is purely kinetic. It results from the active motion and is not due to any particle interactions. The same is true for an enhanced orientational ordering at surfaces, which we also predict together with a strong accumulation of particles, as observed in the experiment [1]. Finally, we extend our analysis to bottom-heavy active particles.

[1] J. Palacci et al. Sedimentation and Effective Temperature of Active Colloidal Suspensions, *Phys. Rev. Lett.*, **105**, 088304 (2010).

(S09 – T5) Brownian particles with active fluctuations

Pawel Romanczuk[1]*, Lutz Schimansky-Geier*[2]
[1] Max Planck Institute for the Physics of Complex Systems, Dresden, [2] Department of Physics, Humboldt-Universität zu Berlin

We study the effect of fluctuating forces on the motion of self-propelled active particles in two spatial dimensions. We distinguish between passive and active forces. Passive fluctuating forces (e.g. thermal fluctuations) are independent of the orientation of the particle. In contrast, active ones point parallel or perpendicular to the time-dependent orientation of the particle. We derive analytical expressions for the speed and velocity distributions for a generic model of active Brownian particles. We obtain speed distributions with non-vanishing probability of speed zero in contrast to the passive case, which correspond to sharply peaked Cartesian velocity distributions at the origin. Finally, we show that such a behavior may also occur in non-Gaussian active fluctuations and discuss the diffusive behavior of self-propelled particles subject to active fluctuations.

(S09 – T6) Transition to collective motion in bacterial colonies as a dynamical self-assembly of self-propelled rods

Fernando Peruani
Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

We argue that the active motion of bacteria combined with volume exclusion effects of their rod-shaped cell body is sufficient to induce collective motion and a rich clustering dynamics on bacterial monolayers. Moreover, this argument suggests the existence of universal clustering properties in bacterial self-organization, particularly on bacterial collective motion. We present experimental evidence that supports this view. Finally, we discuss that the argument also applies to Vicsek-like models and show that the emergence of a scale-free distribution of moving cluster sizes can be used as an alternative definition for collective motion.

(S09 – P1) Superfast catalytic tubular microjet engines

Adithya N. Ananth[1], *Samuel Sanchez*[1], *Oliver G. Schmidt*[1,2]
[1]Institute for Integrative Nanosciences, Leibniz Institute for Solid State and Materials Research Dresden, Helmholzstr.20, Dresden, Germany, [2]Material Systems for Nanoelectronics, Chemnitz University of Technology, Reichenhainer Str. 70, Chemnitz, Germany

There has been an interest to develop engines at micro/nano scale for various applications ranging from sensors, biology and medicine. The ability to maneuver these microjet engines is essential for precise control and efficiency. We have demonstrated that microjet engines fabricated from rolling up nanolayers of Ti/Cr/Pt, with a diameter range form 5-8 µm and 50 µm in length are powered by catalytic decomposition of hydrogen peroxide into water and oxygen [1-6]. The oxygen liberated forms bubbles and pushes the engines in the opposite direction. In this work, we show on/ off control mechanism of microjet engines by temperature variation. The thermal modulation facilitates to acceleration of the microjet engines to higher speed of ca. 200 body lengths per second. In this work we also present reduced fuel concentration of 0.25 %(v/v) hydrogen peroxide for motion of microjet engines by elevating the temperature to 37° C. These results allow reducing toxicity of peroxide fuel towards efficient microjet engines for future biomedical and drug delivery systems.

[1] A. A. Solovev et al., *Small*, **5**, 14, 1688-1692 (2009). [2] A. Solovev et al., *Adv. Funct. Mater*. **20**, 2430–2435 (2010). [3] S. Sanchez et al., *Chem. Commun*., **47**, 698–700, (2011). [4] S. Sanchez et al., *J. Am. Chem. Soc*., **132**, 13144-13145 (2010). [5] S. Sanchez et al., *J. Am. Chem. Soc*., **133**, 701–703 (2011). [6] S. Sanchez et al., *Chem. Commun*., **47**, 698–700, (2011).

(S09 – P2) Theoretical modelling of bacterial motor dynamics

Eva Baresel, *Rudolf Friedrich*
Institute for Theoretical Physics, University of Münster, Germany

The motion of self-propelled flagellated bacteria consists of two different modalities: "running" if all flagella rotate counter-clockwise or "tumbling" if at least one flagellum rotates clockwise [1]. As a model for these bacterial motors we consider the dynamics of an ensemble of swimming objects, which are composed of two rigidly connected point vortices. The single objects are able to show translation or rotation depending on the circulations of the single point vortices. We discuss the collective behaviour for several of these objects and the resulting velocity fields by means of numerical calculations.

[1] H. C. Berg, *Phys. Today*, **53**, 24 (2000).

(S09 – P3) Self-propulsion of a rough Janus particle via a chemical concentration gradient

Pierre de Buyl[1,2], *Raymond Kapral*[1]
[1] Chemical Physics Theory Group, Chemistry Department, University of Toronto,[2] Center for Nonlinear Phenomena and Complex Systems, Université Libre de Bruxelles

Janus particles are two sided objects whose intrinsic asymmetry may be used to generate a gradient around the particles, leading to an effective propulsion [1]. We characterize this motion in the case of a simple catalytic reaction. Mesoscopic hydrodynamical simulations (Multiparticle collision dynamics) coupled to molecular dynamics [2] allow us to study the directed motion within a solvent. The modeling of the Janus particle as an elastic network of beads leads to a microscopic description that includes reactive and nonreactive collisions with the surface beads of the network.

[1] J. R. Howse et al., Self-Motile Colloidal Particles: From Directed Propulsion to Random Walk. *Phys. Rev. Lett.,* **99**, 48102 (2007).

[2] R. Kapral. Multiparticle collision dynamics: simulation of complex systems on mesoscales. *Adv. Chem. Phys.,* **140**, 89 (2008).

(S09 – P4) Energetics of active phoretic motion

Benedikt Sabass, Udo Seifert
II. Institut für Theoretische Physik, Universität Stuttgart, Germany

Small particles, in a viscous medium, producing an asymmetric distribution of solute molecules around them, undergo phoretic motion. The driving force of this motion is the interaction of the solutes with the swimmer via a surface potential.

Here, we first examine the dependence of the phoretic speed on the range of the surface potential and present results for ionic and non-ionic solutes. Next, we discuss the energetics of this active motion [1]. The overall efficiency of a swimmer held by a chemical reaction in a true steady state is calculated. We find that solute convection plays an important role for the thermodynamic picture. Finally, the role of the hydrodynamic efficiency as an upper bound to the overall efficiency is stressed.

[1] B. Sabass and U. Seifert, Efficiency of Surface-Driven Motion, *Phys. Rev. Lett.,* **105**, 218103 (2010).

(S09 – P5) Catalytic and biocatalytic tubular microbots

Samuel Sanchez[1], Alexander A. Solovev[1], Sabine Schulze[1,2], Stefan Harazim[1], Oliver G. Schmidt[1,3]
[1]Institute for Integrative Nanosciences, IFW Dresden, D-01069 Dresden, Germany, [2]Institute of Physiological Chemistry, Medical Faculty Carl Gustav Carus, Dresden University of Technology, Fiedlerstraße 42 D-01307 Dresden, Germany, [3]Material Systems for Nanoelectronics, Chemnitz University of Technology, Reichenhainer Str. 70, D-09107 Chemnitz, Germany

We will review our recent achievements on catalytic and biocatalytic microtubular engines (microbots). These micromachines are fabricated by the well established rolled-up technique developed in our group where different materials can be deposited on Si substrates [1]. In our particular cases, our tubes contain either Au modified with Self-Assembled Monolayers or Pt as inside layer. The microtubes are immersed in hydrogen peroxide as chemical fuel and start to catalytically decompose the peroxide into water and oxygen microbubbles generated in the tubular cavities. Thus, the released bubbles propel the microengine at the liquid-air interface [2]. Moreover, microengines containing a ferromagnetic layer can be externally controlled by magnetic field, which allows the selective manipulation of different microobjects [3] and neuronal cells [4] (Fig.1, right) randomly suspended in solution and therefore used as nanofabrication tools. A more efficient locomotion is achieved by using an enzyme which decomposes peroxide, catalase, and a low concentration of peroxide fuel (1.5 wt %) (Fig.1, Left). The high efficiency of these microengines is of significant importance towards the design of more powerful nanomachines. This is the first report on the effective use of enzymes as catalysts in self-propelled microengines [5]. Finally, we describe the ability of integrate catalytic microengines into microfluidic networks and their magnetic control to guide their motion towards the load and transport of microparticles [6] and cells [7].

[1] O.G. Schmidt and K. Eberl, *Nature*, **410**, 168 (2001); Y. F. Mei et al., *Adv. Mater.* **20**, 4085-4090 (2008).
[2] A. A. Solovev et al., *Small*, **5**, 14, 1688-1692 (2009).
[3] A. Solovev et al., *Adv. Funct. Mater.* **20**, 2430–2435 (2010).
[4] S. Sanchez et al., *Chem. Commun*., **47**, 698–700, (2011).
[5] S. Sanchez et al., *J. Am. Chem. Soc.*, **132**, 13144-13145 (2010).
[6] S. Sanchez et al., *J. Am. Chem. Soc.*, **133**, 701–703 (2011).
[7] S. Sanchez et al., *Chem. Commun*., **47**, 698–700, (2011).

(S09 – P6) Dynamics of a deformable self-propelled particle under external forcing

Mitsusuke Tarama and Takao Ohta
Department of Physics, Kyoto University, Kyoto, 606-8502, Japan

We have investigated dynamics of a self-propelled deformable particle under external field in two dimensions based on the model equations for the center of mass and a tensor variable characterizing deformations. Here, we have considered two kinds of external force. One is a gravitational-like force, which enters additively in the time-evolution equation for the center of mass. The other is an electric-like force supposing that a dipole moment is induced in the particle. This force is added to the equation for the deformation tensor. The system we consider is simply a single isolated particle but has internal degrees of freedom due to deformability. It should be noted that, even when the external forcing is absent, there is a bifurcation between a straight motion and a rotating motion [1]. Therefore, by adding an external force, there occurs a conflict or frustration between the rotating motion and the forced straight motion. As a result, non-trivial states of motion and bifurcations are exhibited by changing the magnitude of the external force. We have carried out numerical simulations of the time-evolution equations to obtain a dynamical phase diagram. Analytical study has also been developed to reproduce some of the bifurcations.

[1] T. Ohta and T. Ohkuma, *Phys. Rev. Lett.*, **102**, 154101 (2009).
[2] M. Tarama and T. Ohta, (submitted to EPJB).

Symposium 10: **Applications to Cell Biology**

(S10– I) Introduction

M. Falcke
Max-Delbrück-Center for Molecular Medicine, Berlin, Germany

(S10– T1) Spatial phase singularities and cell shape dynamics

Satoshi Sawai[1,2]
[1] Graduate School of Arts and Sciences; [2] Research Center for Complex Systems Biology, University of Tokyo

It has been shown that Phosphatidylinositol (3,4,5)-triphosphate (PIP3) self-organizes into propagating waves that induce membrane protrusions during spontaneous cell migration in *Dictyostelium discoideum* cells. We show how geometry of PIP3 waves appear to determine timing, direction and shape of large-scale membrane protrusions. Specifically, we address the origins and the dynamics of phase singularities to clarify the kinematics of cell shape change. A single isolated phase singularity near the cell edge supported a single-arm spiral wave that results in rotational membrane protrusions, whereas a pair of singularities gave rise to a planar wave that pushed the membrane towards the cellular edge. When a new wave front appears at a rear side of an existing wave, a pair of new singularities are created by means of type-zero phase resetting. We have studied these properties by constructing a mathematical model of a simple reaction-diffusion scheme coupled to dynamics of membrane deformation. The observed F-actin dependence of the nucleation rate and propagation of PIP3 waves suggests actin-dependent feedback regulation of PIP3 whose strength determines the threshold for excitation and stability of the fixed points in the dynamics. I will also discuss the relation between the observed spontaneous pattern generation at the single cell-level and the spatio-termporal patterns of chemoattractant field at the multi-cellular level [1,2].

[1] T. Gregor, N. Masaki, K. Fujimoto & S. Sawai. The onset of collective behavior in social amoebae. *Science* **328**, 1021-1025 (2010).
[2] S. Sawai, P.Thomason & E. C. Cox. An autoregulatory circuit for long-range self-organization in *Dictyostelium* cell populations. *Nature* 433, 323-326 (2005).

(S10– T2) Inherent polarity and gradient sensing of the self-organized signaling system in chemotactic cells

Tatsuo Shibata
Laboratories for Physical Biology, RIKEN Center for developmental biology 2-2-3 Minatojima-minamimachi, Chuo-ku, Kobe 650-0047, Japan, and PRESTO, Japan Science and Technology Agency (JST), 4-1-8 Honcho Kawaguchi, Saitama, Japan

The phosphatidylinositol (PtdIns) lipids reaction is a key signaling event responsible for gradient sensing for eukaryotic cell chemotaxis. The self-organization activity of the PtdIns lipids reaction induces an inherent polarity even in the absence of an external chemoattractant gradient by producing a localized domain of PI(3,4,5)P3 on the membrane. We found experimentally that such a domain can exhibit two kinds of behavior: 1) persistent domain formation that travels on the membrane over time [1], and 2) stochastic formation of transient domains. The enzymes phosphatase and tensin homolog (PTEN) and phosphoinositide-3-kinase (PI3K), which are regulators for PtdIns lipid concentrations along the membrane, were essential for self-organization behaviors whereas functional actin cytoskeleton was not. Defects in these enzymes inhibited such a behavior. We then developed a statistical method to reconstruct a phase portrait of the characteristic dynamics of the PtdIns lipids system from the noisy time-lapse data of fluorescent images of each single cell. On the basis of the experimental results and the reconstructed dynamics, we developed a theoretical model for the PtdIns lipids signaling system, which can reproduce both behaviors; oscillatory and excitability properties of the system explaining each, respectively. Further analysis indicates that this self-organized system responds sharply to a shallow external gradient by modulating the precision of domain position and formation frequency. These results imply that the self-organized activity, independent of external cues, is the basis for sensitivity to shallow chemoattractant gradients.

[1] Y. Arai, T. Shibata, S. Matsuoka, M. J. Sato, T. Yanagida, and M. Ueda, Self-organization of the phosphatidylinositol lipids signaling system for random cell migration. *PNAS,* **107**, 12399-12404 (2010).

(S10– T3) Cellular polarization by coupling an active fluid to a pattern forming system

Stephan W. Grill[1,2]
[1] Max Planck Institute for Molecular Cell Biology and Genetics, Dresden, Germany, [2] Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

I will present recent advances of our understanding of coupling of mechanical and biochemical processes to enact morphologic change in biological systems. I will discuss the mechanism of pattern formation in active fluids in which active stress is regulated by diffusing molecular components [1]. Nonhomogeneous active stress profiles create patterns of flow, which transport stress regulators by advection. I apply this framework to the polarization of the *C. elegans* zygote, a classic example of mechanochemical coupling. Here, a conserved network of PAR polarity proteins segregate themselves into an anterior and a posterior domain. Here we present evidence that PAR polarity arises from coupling of an actin-independent PAR reaction-diffusion system with passive advective transport of PARs by a mechanically active and flowing cell cortex [2]. Our experimental and theoretical findings show that advection is sufficient to account for the initial segregation of anterior PAR proteins, and that this segregation can serve to trigger pattern formation within an otherwise stable, unpolarized PAR system. This work suggests that passive advective transport in a regulated active material is a general mechanism by which patterns are established in developmental systems.

[1] J. S. Bois, F. Jülicher S. W. Grill, Pattern formation in active fluids, *Phys. Rev. Lett.* **106**, 28103 (2011).
[2] N. Goehring, C. Hoege, S. W. Grill, A. A. Hyman, PAR proteins diffuse freely across the anterior-posterior boundary in polarized C. elegans embryos, *J. Cell Biol.*, **193**, 583-594 (2011).

(S10 – P1) *In vivo* characterization of enzymatic networks dynamics

Helene Berthoumieux[1], *Annie Lemarchand*[2], *Charlie Gosse*[3], *K. Zrelli* [4], *T. Le Saux*[4], *Ludovic Jullien*[4]
[1] Biophysics, Physics of Complex Systems, Max Planck Institute, Dresden, [2] Laboratoire de Physique Theorique de la Matiere Condensee, Paris06, UMR CNRS-UPMC 7600, [3] Laboratoire de Photonique et de Nanostructures, LPN-CNRS [4] Departement de Chimie, ENS, UMR CNRS-ENS-UPMC Paris 06 8640 Pasteur

Biologists, biophysicists and chemists are interested in the description of biochemical species and in the copy of their dynamical properties. For a good characterization of the kinetics of such objects, an *in situ* investigation is essential. During the last 20 years, efficient *in vivo* reporters have been developed and used for the study of the gene regulation pathways. The characteristic time of a transcription process is about half an hour. Our goal is to furnish theoretical and technical tools to investigate the short time scale response of the cell, i.e. from the millisecond to the minute. It involves cascades of fast reactions occurring in the cytoplasm and the characterization of such networks implies the determination of their topology [1], the values of the associated rate constants and the nature of the steady state [2]. We show that this information can be extracted from the response of a species involved in a network to a temperature modulation. We propose protocols to distinguish between different topologies and to determine the value of the rate constants of a given topology. In parallel we design a micro-device that allows to impose controlled temperature modulations [3].

[1] H. Berthoumieux, A. Lemarchand, L. Jullien, *Phys. Rev. E*, **76**, 056112 (2007).
[2]H. Berthoumieux, C. Antoine, A. Lemarchand, *J. Chem. Phys.*,**131**,084106 (2009).
[3] K. Zrelli,T. Barilero, H. Berthoumieux, E. Cavatore, T. Le Saux, V. Croquette, A. Lemarchand, C. Gosse, L. Jullien, *Anal. Chem.,* **83**, 7 (2011).

(S10 – P2) Predicting the impact of mutations on the stability and on the thermal resistance of protein structures

Yves Dehouck [1,2], *Benjamin Folch*[1], *Dimitri Gili*[1], *Marianne Rooman*[1]
[1] Genomic and structural Bioinformatics, Université Libre de Bruxelles, Belgium, [2] Fritz-Haber-Institut der Max-Planck Gesellschaft, Germany

The ability to model and predict of the effect of mutations in proteins is highly valuable in the context of the rational design of modified proteins with controlled properties, the guidance of experimental studies of protein structure and function, and the rationalization of the effect of naturally occurring variants (eg. disease-causing mutations). We present a method for the prediction of stability changes induced by mutations in proteins, which relies on a combination of statistical potentials extracted from a dataset of know protein structures [1]. The possibility of describing effectively the temperature dependence of the interactions that govern protein stability was also investigated, in view of improving the prediction of the thermal resistance of mutated proteins [2].

[1] Y. Dehouck, A. Grosfils, B. Folch, D. Gilis, Ph. Bogaerts, M. Rooman, *Bioinformatics*, **25**, 2537 (2009).
[2] B. Folch, M. Rooman, Y. Dehouck, *J Chem Inf Model*, **48**, 119 (2008); B. Folch, Y. Dehouck, M. Rooman. *Biophys J*, **98**, 667 (2010).

(S10–P3) Elastic-network study of intramolecular communication in myosin-V

Markus Düttmann[1], *Yuichi Togashi*[2,3], *Toshio Yanagida*[3,4], *Alexander Mikhailov*[1]
[1] Department of Physical Chemistry, Fritz Haber Institute of the Max Planck Society, Berlin, [2] Applied Information Systems Division, Cybermedia Center, Osaka University,[3] Quantitative Biology Center, RIKEN,[4] Soft Biosystem Group, Graduate School of Frontier Biosciences, Osaka University

Myosin-V can be described in terms of its functional units: the tail, the nucleotide-binding pocket and the actin-binding cleft. We analyzed communication between these regions in the framework of a coarse-grained elastic network model. Our analysis reveals that when backward or forward strains are applied to the tail, these lead to changes in the actin cleft, which may favor or hinder strong actin binding. Furthermore, external forces affect the opening of the front door and, thus, provide a mechanism to regulate ADP affinity. We could further identify sensitive residues inside the nucleotide-binding pocket. Perturbations in the back-door region induce conformational changes in the actin cleft, while forces applied to residues gating the front door invoke a definite response of the tail. Another group of sensitive residues is located in the so-called hypertrophic cardiomyopathy (HCM) loop, known to be involved in the binding to actin. Application of forces in this are induces motion of the tail and changes in the front-door region.

(S10–P4) A model for the actin-based propulsion of spatially extended objects

Mihaela Enculescu[1], *Martin Falcke*[2]
[1] Institute for Theoretical Physics, Technical University of Berlin,[2] Mathematical Cell Physiology, Max-Delbrück-Centre for Molecular Medicine

A key step of cell migration is the protrusion of the cell membrane through the growth of an actin network that pushes the leading edge. We have proposed a model for simulating the leading edge dynamics of a migrating cell from the interplay among elastic properties and architecture of the actin cytoskeleton and the mechanics of the membrane [1]. Our approach is based on the description of the length and attachment dynamics in the actin network. The model reproduces the marked state switches in protrusion morphodynamics found experimentally between epithelial cells in control conditions and cells expressing constitutively active Rac, a signaling molecule involved in the regulation of actin network assembly. The model can be also adapted to the motion of protein-coated hard beads in a cell-like medium and can explain the experimentally observed transitions of the dynamic regime with changing bead radius and protein surface density [2].

[1] M. Enculescu, M. Sabouri-Ghomi, G. Danuser, M. Falcke. Modeling of Protrusion Phenotypes Driven by the Actin-Membrane Interaction, *Biophys. J.,* **98**, 1-11 (2010).

[2] M. Enculescu, M. Falcke. Actin-based propulsion of spatially extended objects, *New Journal of Physics*, in press (2011).

(S10–P5) Tracing entire operation cycles of molecular motor hepatitis C virus helicase in structurally resolved dynamical simulations

Holger Flechsig and Alexander S. Mikhailov
Department of Physical Chemistry, Fritz Haber Institute of the Max Planck Society Berlin, Faradayweg 4-6, 14195 Berlin, Germany

Hepatitis C virus helicase is a molecular motor that splits duplex DNA while actively moving over it. An approximate coarse-grained dynamical description of this protein, including its interactions with DNA and ATP, is constructed. Using such a mechanical model, entire operation cycles of an important protein machine could be followed in structurally resolved dynamical simulations. Ratcheting inchworm translocation and spring-loaded DNA unwinding, suggested by experimental data, were reproduced. Thus, feasibility of coarse-grained simulations, bridging a gap between full molecular dynamics and reduced phenomenological theories of molecular motors, has been demonstrated [1].

[1] H. Flechsig, A.S. Mikhailov. Tracing entire operation cycles of molecular motor hepatitis C virus helicase in structurally resolved dynamical simulations. *Proc. Natl. Acad. Sci. USA*, **107**, 20875 (2010).

(S10 – P6) Spiral-wave prediction in a lattice of FitzHugh-Nagumo oscillators

Miriam Grace and Marc-Thorsten Hütt
School of Engineering and Science, Jacobs University Bremen, Bremen, Germany

In many biological systems, variability of the components can be expected to outrank statistical fluctuations in the shaping of self-organized patterns. The distribution of single-element properties should thus allow the prediction of features of such patterns. In a series of previous studies on established computational models of *Dictyostelium discoideum* pattern formation we demonstrated that the initial properties of potentially very few cells have a driving influence on the resulting asymptotic collective state of the colony [1,2]. One plausible biological mechanism for the generation of variability in cell properties and of spiral wave patterns is the concept of a 'developmental path', where cells gradually move on a trajectory through parameter space. Here we present an analogous one-dimensional developmental path based on the FitzHugh-Nagumo model, incorporating parameter drift and concomitant variability in the distribution of cells embarking on this path, which gives rise to stable spiral waves. We anticipate that such a generic model of spiral wave predictability will allow new insights into the relationship between properties of the variability of the initial cellular constituents and features of the resulting spatiotemporal pattern.

[1] Geberth, D. and Hütt, M.-Th. (2008) Predicting spiral wave patterns from cell properties in a model of biological self-organization. *Phys. Rev. E,* **78**, 031917.

[2] Geberth, D. and Hütt, M.-Th. (2009) Predicting the distribution of spiral waves from cell properties in a developmental-path model of *Dictyostelium* pattern formation. *PLoS Comput. Biol.,* **5**, e1000422.

(S10 – P7) Weber's law in autocatalytic reaction networks

Masayo Inoue[1], *Kunihiko Kaneko*[2]
[1] Cybermedia Center, Osaka University, [2] Department of Basic Science, University of Tokyo

Biological responses often obey Weber's law, according to which the magnitude of the response depends only on the fold change in the external input. In this study, we demonstrate that a system involving a simple autocatalytic reaction shows such response when a chemical is slowly synthesized by the reaction from a faster influx process. We also show that an autocatalytic reaction process occurring in series or in parallel can obey Weber's law with an oscillatory adaptive response. Considering the simplicity and ubiquity of the autocatalytic process, our proposed mechanism is thought to be commonly observed in biological reactions.

(S10 – P8) Intrinsic heterogeneity in the phosphatidylinositol response against cAMP in Dictyostelium discoideum

Masatoshi Nishikawa[1,2], *Masahiro Ueda*[2,3], *Tatsuo Shibata*[1,2]
[1] Laboratories for Physical Biology, RIKEN Center for developmental biology, [2] Japan Science and Technology Agency

(JST), CREST, [3] Laboratory for Cell Signaling Dynamics,RIKEN Quantitative biology center
Phosphatidylinositol 3,4,5-trisphosphate (PtdIns(3,4,5)P3) has been shown to be a key signaling molecule of random cell migration as well as of chemotactic movement for cAMP in *Dictyostelium discoideum*. Even in the absence of explicit chemoattractant stimulus, we found the transient formation of localized PtdIns(3,4,5)P3 accumulating domain on the membrane. The formation of PtdIns(3,4,5)P3 enriched domain are accompanied with the decrease of PTEN concentration on the membrane which catalyzes PtdIns(3,4,5)P3 dephosphorylation. These bursts of PtdIns(3,4,5)P3 result in the spatial distribution of PtdIns(3,4,5)P3 and PTEN to be heterogeneous. Such a spatial heterogeneity of signaling molecules could affect the cAMP response. In the present study, we first show the transient response of PtdIns(3,4,5)P3 by the step increase of cAMP concentrations, and found that the response is spatially localized against the small increase of cAMP concentration. While the PtdIns(3,4,5)P3 response averaged over the whole membrane area is proportional to the cAMP concentration, the amplitude of PtdIns(3,4,5)P3 burst in responded region is independent of the cAMP concentration. We then show that transient increase of cAMP concentration is sufficient to trigger the PtdIns(3,4,5)P3 burst. Once a PtdIns(3,4,5)P3 response is initiated, the amplitude of the burst is similar to that by the step stimulus, indicating that the PtdIns(3,4,5)P3 burst is generated by the excitable dynamics.

(S10 – P9) Spatial modeling of calcium release puffs

Sten Rüdiger
Institut für Physik, Humboldt University, Newtonstr. 15, 12489 Berlin
I describe recent work on the cooperativity of calcium releasing channels in the interior of cells. Hybrid stochastic-deterministic simulations were used to calculate spatial distributions of calcium within clusters of channels. In general, diffusion of calcium between channels and stochastic binding of calcium to activating channel sites leads to random but cooperative openings of channels. I show that for these so-called puffs the mixing assumption for reactants does not hold within the clusters. Consequently, the law of mass action does not apply and useful definitions of averaged calcium concentrations in the cluster are not obvious. Effective reaction kinetics can be derived, however, by separating concentrations for self-coupling of channels and coupling to different channels. Based on the spatial approach, a minimal Markovian model can be inferred, describing well calcium puffs in neuronal cells and allowing insight into the mechanism of calcium puffs.

Symposium 11: **Stochastic Theory of Chemical Reactions**

(S11 – I) Introduction

Igor Sokolov[1] and K. Lindenberg[2]
[1] Dept. of Physics, Humboldt-University Berlin, Germany, [2] Dept. of Chemistry and Biochemistry, University of California San Diego,
La Jolla, CA, USA

(S11 – T1) Stochastic chemical kinetics

Dan Gillespie
Dan T. Gillespie Consulting, 30504 Cordoba Pl., Castaic, CA 91384, USA
The time evolution of a well-stirred chemically reacting system is traditionally modeled by a set of coupled ordinary differential equations called the reaction rate equation (RRE). The resulting picture of continuous deterministic evolution is, however, valid only for infinitely large systems. That condition is usually well approximated by test tube size systems. But in biological systems formed by single living cells, the small molecular populations of some reactant species can result in dynamical behavior that is noticeably discrete rather than continuous, and stochastic rather than deterministic. In that case, a physically more accurate mathematical modeling is obtained by using the machinery of Markov process theory, specifically, the chemical master equation (CME) and the stochastic simulation algorithm (SSA). In this tutorial talk, we will first review the theoretical foundations of stochastic chemical kinetics. Then we will derive some approximate accelerated simulation procedures that turn out to form a logical bridge from the discrete-stochastic CME/SSA formalism to the continuous-deterministic RRE formalism.

(S11 – T2) Enhancement of electrochemical reaction rates at the nanoscale, loss of correlations in electrochemical oscillators and superstatistics

Vladimir García-Morales[1,2], Katharina Krischer[1]
[1] Physik Department E19a, Technische Universität München, Garching, [2] Institute for Advanced Study, Technische Universität München, Garching
Considering chemical systems, the evolution of the number of reacting chemical species in a small volume is described by the chemical master equation [1] which can be simulated by the Gillespie's algorithm [2] In electrochemical nanosystems, we have recently shown [3] that the stochasticity of electron transfer events on a resistively coupled nanoelectrode causes mesoscopic fluctuations of the electrode potential. These fluctuations give rise to a time-average

faradaic current density substantially larger than in the macroscopic limit. The deviations result to a large extent from the external, potentiostatic control, which imposes a constraint on the evolution of the electrode potential. The degree of freedom of the electrode potential requires a resistance between nanoelectrode and metallic support. The resulting stochastic electrochemical steps are non-Markovian because of this external control. In this talk, the tools to simulate such electrochemical nanosystems will be presented. We introduce an electrochemical master equation consisting on the chemical master equation coupled to the stochastic dynamics of the electrode potential, on which the reaction rates depend exponentially [3]. At the stationary state, we find distributions that are long-tailed (rare events are favored) compared to the normal distributions found in chemical systems. These long tails have a strong influence in the enhanced electrochemical kinetics found at the nanoscale. In the limit of infinite electrode size, the normal distributions of standard statistical mechanics are regained. We will discuss also the effects of molecular noise on the loss of correlations in oscillatory electrochemical reaction networks at the nanoscale. Finally, a connection of the statistics of nanoscale electrochemical systems and superstatistics (Tsallis entropy) will be discussed.

[1] P. Gaspard, *J. Chem. Phys.,* **117,** 8905 (2002).
[2] D.T. Gillespie, *J. Phys. Chem.,* **81,** 2340 (1977).
[3] V. Garcia-Morales and K. Krischer, *Proc. Natl. Acad. Sci., USA* **107,** 4528 (2010).

(S11 – T3) Reliable information processing in noisy intracellular networks

Tetsuya. J. Kobayashi, *Atsushi Kamimura*
Institute of Industrial Science, the University of Tokyo

While using intrinsically stochastic intracellular reactions as the building components, cellular systems can make adaptive response robustly in the ever-changing environment in sharp contrast with man-made systems whose robust operation usually depend on the reliability of their components. This fact strongly suggests that certain structures of intracellular networks implement dynamical mechanism that can compensate the noise, which is yet to be fully revealed. In this work, we show that several intracellular networks such as phosphorylation cycles with auto-regulatory feedback can implement Bayesian information decoding, which enables a cell to extract information from noisy signal and to make appropriate response subsequently [1,2]. This information decoding dynamics is further revealed to have a tight connection with noise-induced symmetry-breaking phenomenon [3], in which distinct macroscopic output is generated not by deterministic symmetry-breaking by noise. The underlying principle of this robust information processing is also clarified to be exploitation of infinite-dimensionality of temporal dynamics.

[1] T.J.Kobayashi, Implementation of dynamic Bayesian decision making by intracellular kinetics. *Phys. Rev. Lett.*, **104**, 228104 (2010).
[2] T.J.Kobayashi, A.Kamimura. Dynamics of intracellular decision making and its statistical principle. *Phys. Biol.*, submitted (2011).
[3] T.J.Kobayashi, Connection between noise-induced symmetry-breaking and information decoding function for intracellular networks. *Phys. Rev. Lett.*, in press (2011).

(S11 – T4) Effects of internal noise in mesoscopic chemical oscillation systems: The stochastic normal form theory

Zhonghuai Hou
Department of Chemical Physics & Hefei National Lab for Physical Science at Microscales, University of Science and Technology of China, Hefei, Anhui, 230026, P.R.China

Effects of internal noise in mesoscopic chemical osicllation systems have gained much attention in recent years. In the vicinity of the deterministic supercritical Hopf bifurcation where the stable limit cycle emerges, noise can induce sustained oscillations outside the deterministic oscillatory region. In addition, the performance of the noise induced oscillation (NIO), characterized by a well-defined signal-to-noise ratio, shows a clear-cut maximum with the variation of the internal noise intensity, a phenomenon known as internal noise coherence resonance (INCR). Since the magnitude of the internal noise is inversely proportional to the system size, the INCR also indicates a kind of optimal system size effect [1-2]. Simulations showed that this phenomenon is quite common in small chemical oscillation systems [3-5]. To understand the underlying mechanism of this interesting phenomenon, we have developed an analytical theory, the stochastic normal form theory (SNFT) [6-7], which can not only explain the INCR very well, but also can provide new insights into the roles of internal noise [8]. By using this theory, we can also study the issue of stochastic thermodynamics and fluctuation theorems in mesoscopic oscillation systems. The analysis showed that the entropy production along a stochastic limit cycle, as a function of the system size V, shows distinct scaling laws with V at different side of the Hopf bifurcation [9-10].

[1] Z. Hou and H. Xin. Internal Noise Stochastic Resonance in a Circadian clock System. J. Chem. Phys. **119** (22), 11508 (2003).
[2] Z. Hou and H. Xin. Optimal System Size for Mesoscopic Chemical Oscillations. *ChemPhysChem* **5**, 407(2004).
[3] Y. Gong, Z. Hou, and H. Xin. Optimal particle size for reaction rate oscillation in CO oxidation on nm-sized palladium particles. *J. Phys. Chem. B,* **108**, 17796 (2004).
[4] Z. Hou and H. Xin. Effects of Internal Noise for Rate Oscillations During CO Oxidation on Platinum Surfaces. *J. Chem. Phys.,* **122**, 134708 (2005).

[5] H. Li, Z. Hou, and H. Xin. Internal Noise Stochastic Resonance for Intracellular Calcium Oscillation in a Cell System. *Phys. Rev. E,* **71**, 061916 (2005).
[6] Z., J. Xiao, and H. Xin. Internal noise coherent resonance for mesoscopic chemical oscillations: A fundamental study. *ChemPhysChem,* **7**, 1520 (2006).
[7] T. Xiao and J. Ma, Zhonghuai Hou, Houwen Xin. Effects of internal noise in mesoscopic chemical systems near Hopf bifurcation. *New. J. Phys.,* **9**, 403 (2007).
[8] J. Ma, T. Xiao, Z. Hou, and H. Xin. Coherence Resonance Induced by Colored Noise near Hopf Bifurcation. *Chaos,* **18**, 043116 (2008).
[9] T. Xiao, Z. Hou, and H. Xin. Entropy production and fluctuation theorem along a stochastic limit cycle. *J. Chem. Phys.,* **129**, 114506 (2008).
[10] T. Xiao, Z. Hou, and H. Xin. Stochastic thermodynamics in mesoscopic chemical oscillation systems. *J. Phys. Chem. B,* **113**, 9316 (2009).

(S11 – T5) Utilizing history for robust information processing by intracellular reactions

Atsushi Kamimura, Tetsuya J. Kobayashi
Institute of Industrial Science, The University of Tokyo, Japan

Inherently stochastic character of chemical reactions results in very noisy cellular processes. While recent direct experimental observations support this, it suggests that they are different from conventional human-made machineries in which noise usually prevents from precise information transmission and processing. One possible way to keep the consistency between their robust responses and apparent noisy signals is that cells utilize the information not only of instantaneous signals but also of their histories. However, it is not fully understood what kind of structures and mechanisms of chemical reactions can exploit the information that the history has. To address this problem, we point out here, in the processing flow from environmental signals to intracellular networks, reconstructing information of the starting point is possible at the end point of the flow, by using the temporal history of signals, even though instantaneous signals at the intermediate steps are very noisy [1]. In particular, we clarify that, by measuring mutual information, certain structure of reactions, which can implement dynamic Bayesian information processing, determines the maximum limit of such decoding. In addition to the temporal processing, we also consider spatial degree of freedom concerning statistics, to investigate collective effects for robust responses.

[1] T. J. Kobayashi and A. Kamimura, Dynamics of intracellular decision making and its statistical principle, *Phys. Biol.*, submitted (2011).

(S11 – P1) Master equation simulation of FKPP front: effect of perturbed particle velocity distribution

Piotr Dziekan[1], Bogdan Nowakowski[1], Annie Lemarchand[2,3]
[1] Institute of Physical Chemistry, 01-224 Warsaw, Poland, [2] Université Pierre et Marie Curie - Paris 6, LPTMC, France
[3] CNRS, LPTMC UMR 7600, Paris, France

We develop a master equation for reaction-diffusion processes including the corrections due to the perturbation of the particle velocity distribution by the chemical reaction. Simulations of the mesoscopic dynamics based on the modified master equation are performed for the FKPP chemical wavefront [1]. Significant deviations are observed for the speed and width of the front with respect to the results of the macroscopic reaction-diffusion equation without nonequilibrium corrections. The results at the mesoscopic level agree with microscopic simulations obtained by means of the direct simulation Monte Carlo method for dilute gases.

[1] J. S. Hansen, B. Nowakowski, and A. Lemarchand, J. Chem. Phys. **124**, 034503 (2006).

(S11 – P2) Stochastic birth and death processes including delay

Luis F. Lafuerza, Raul Toral
IFISC, Institute for Cross-Disciplinary Physics and Complex Systems, CSIC-UIB, Spain

Motivated by gene regulation where elementary processes such as transcription and translation take a finite time to be completed, and the whole process is significantly stochastic, we consider stochastic birth and death processes that explicitly include time delays. In the case of delayed production with negative feedback we show that the fluctuations change from sub-Poissonian to super-Poissonian as the delay is increased, so that a negative feedback decreases or increases the fluctuations depending on the magnitude of the delay. In the case of delayed degradation we solve the process exactly and show that, contrary to previous results, stochastic oscillations are not present and that the system has always Poissonian character.

(S11 – P3) Constructive role of internal fluctuations on axial segmentation

Annie Lemarchand[1], Bogdan Nowakowski[2]
[1] Laboratoire de Physique Théorique de la Matière Condensée, Université Pierre et Marie Curie – CNRS, 4 Place Jussieu, case courrier 121, 75005 Paris, France, [2] Institute of Physical Chemistry, Polish Academy of Sciences, ul. Kasprzaka 44/52, 01-224 Warszawa, Poland

In biology, axial segmentation refers to the formation of a periodic pattern along the antero-posterior axis of some animals, such as arthropods, annelids and vertebrates [1]. The deterministic approach to the reaction-diffusion model we have developed reproduces the main features of axial segmentation observed during morphogenesis: The numerical integration of the deterministic equations for the concentrations gives account for the passage of a wave front, first followed by damped time oscillations and then by the formation of a stationary periodic spatial structure for appropriate parameter values. The stochastic description, possible thanks to the foundation of the model on explicit microscopic processes, shows that the internal fluctuations, instead of blurring the spatial pattern, accelerates its formation just after the passage of the wave front, sustains it in regions of the medium where it is not predicted by the deterministic description and extends the parameter domain where it exists. In the framework of this reaction-diffusion model, the development of axial segmentation is definitely favored by the internal fluctuations [2].

[1] A. Aulehla, W. Wiegraebe, V. Baudet, M. B. Wahl, C. Deng, M. Taketo, M. Lewandoski, and O. Pourquié, *Nat. Cell. Biol.,* **10**, 186 (2008).
[2] A. Lemarchand and B. Nowakowski, *Europhys. Lett.*, **94** (4), 48004 (2011).

Symposium 12: **Networks**

(S12 – I) Introduction

S. Bornholdt
Department of Physics, University of Bremen, Germany

(S12 – T1) Engineering self-organized criticality in adaptive networks

Anne-Ly Do, and Felix Droste, Thilo Gross
Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

Many information processing systems are known operate at maximal efficiency when their parameters are tuned to a critical where a phase transition occurs. Perhaps the most fascinating example of computation at criticality is found in the brain, for which the “criticality hypothesis”[1] is presently supported by increasing empirical evidence. This raises the question how a complex biological system, such as the brain, can remain close to the critical state despite ongoing changes due to development, adaptation and aging. A likely answer is found in adaptive networks [2], a new class of models combing topological evolution of a network and dynamics of a network. Several previous works [3,4,5] demonstrated that adaptive networks can self-organize robustly to critical states based on simple local rules. In the present talk we first illustrate the mechanism of adaptive self-organized criticality in a simple, analytically-tractable model. Extrapolating from the simple example, we then discuss perspectives for engineering adaptive self-organized criticality in technical systems.

[1] J.M. Beggs: The criticality hypothesis, *Phil. Trans. Roy. Soc. A,* **336**, 329 (2008).
[2] T. Gross and B. Blasius, Adaptive Networks: A Review, *J. Roy. Soc. Interface,* **5**, 259 (2007).
[3] S. Bornholdt and T. Rohlf, Global Criticality from Local Dynamic, *Phys. Rev. Lett.,* **84**, 6114 (2000).
[4] A. Levina, J.M. Herrmann, T. Geisel, Phase Transitions towards Criticality in a Neural System with Adaptive Interactions, *Phys. Rev. E,* **102**, 118110 (2009).
[5] C. Meisel and T. Gross, Adaptive self-organization in a realistic neural network model, *Phys. Rev. E*, **80**, 061917 (2009).

(S12 – T2) Attractor and basin entropies of random Boolean networks under asynchronous stochastic update

Jörn Davidsen[1], Amer Shreim[1], Andrew Berdahl[1,2], Florian Greil[1,3], Maya Paczuski[1]
[1] Complexity Science Group, Department of Physics & Astronomy, University of Calgary, Canada, [2] Department of Ecology & Evolutionary Biology, Princeton University, Princeton, USA, [3] Arbeitsgruppe Komplexe Systeme, Institut für Festkörperphysik, Technische Universität Darmstadt, Germany

One of the main challenges in biological sciences is to identify regulatory networks from high-throughput experiments. Relevant criteria for models include conceptual simplicity, computational tractability, and robustness to uncertainties in the data. Boolean networks are candidates for representing classes of behaviors observed in large regulatory networks. In contrast to what is often assumed when studying Boolean networks, many real world systems do not evolve according to a globally synchronized clock. Here, we introduce a method to study random Boolean networks with asynchronous stochastic update. Each node in the state space network starts with equal occupation probability, which then evolves to a steady state. Attractors and the sizes of their basins are determined by the nodes left occupied at late times. While most properties differ drastically from the case of synchronous update including the distribution for the number of attractors and basin sizes, the basin entropy grows with system size only for critical networks in both cases. Hence, it is a robust and unambiguous detector of critical behavior.

(S12 – T3) Uncovering the hidden geometry behind metabolic networks

Marián Ángeles Serrano[1], Marián Boguñá[2], Francesc Sagués[1]
[1] Departament de Química Física, Universitat de Barcelona, Spain, [2] Departament de Física Fonamental, Universitat de Barcelona, Spain

Hidden geometries underlying some real complex networks appear to provide a simple and natural explanation for their observed topological properties. The underlying metric spaces can range from hierarchical random graphs, very flexible random tree models that can be adapted to generate a wide variety of topological features, to the S1 model, an euclidean one-dimensional model that is able to reproduce the topological self-similarity observed in many real networks [1]. Beyond the ability of these models to simulate the observed topologies, they enable an inverse method to map real complex networks to congruent metric spaces. This mapping brings new insights into how different subparts of the network relate to each other. In this talk, we apply these ideas to metabolic networks in the cell. Metabolism, the set of biochemical reactions that secure life, admits a bipartite network representation, with metabolites and reaction as nodes, that can be successfully embedded into a metric space. To solve the inverse problem, we consider two different metric spaces and two of the most distinctive network reconstructions that can be found in available databases, human and *E. coli* metabolisms. We use hierarchical random graphs to define reaction scores that assess the likelihood of each reaction in probabilistic terms. This network-based scoring system uncovers very specific reactions that could be functionally or evolutionary important, identifies prominent experimental targets, enables further confirmation of modeling results, and complements the currently employed confidence scores that rate reactions according to experimental evidence [2]. Over and above, the S1 model turns out to be an outstanding paradigm for the analyzed metabolic networks. Using its simple and intuitive geometry of a circle, the notion of biochemical pathway acquires a renewed perspective that unveils the organization of the higher hierarchical levels in metabolic networks based on the concept of cross-talk between pathways [3].

[1] M. A Serrano, D. Krioukov, M. Boguñá. Self-similarity of complex networks and hidden metric spaces, *Phys. Rev. Lett.*, **100**, 078701 (2008).

[2] M. A Serrano, F. Sagués. Network-based scoring system for genome-scale metabolic reconstructions, *arXiv:1008:3166, under review BMC Systems Biology.*

[3] M. A Serrano, M. Boguñá, F. Sagués. Uncovering the hidden geometry behind metabolic networks: from molecular interactions to cross-talks between pathways, *in preparation.*

(S12 – T4) Network structure dependence of oscillation regularity in coupled noisy oscillators

Hiroshi Kori[1, 2], *Yoji Kawamura*[3], *Naoki Masuda*[4, 2]

[1] Division of Advanced Sciences, Ochanomizu Univeristy, Tokyo, Japan [2] PRESTO, Japan Science and Technology Agency, Kawaguchi, Japan [3] Institute for Research on Earth Evolution, Japan Agency for Marine-Earth Science and Technology, Yokohama, Japan, [4] Graduate School of Information Science and Technology, The University of Tokyo, Tokyo, Japan

Biological pacemaker organs are composed of oscillatory cells. Examples include the circadian master clock and the heart pacemaker. Although cells are subjected to external or intrinsic noise, pacemaker organs are capable of forming regular oscillations, i.e., small standard deviation (SD) of cycle-to-cycle periods. We study a network of noisy phase oscillators and obtain an expression for the dependence of the SD on network parameters, such as coupling strength, network connectivity and network size N. We find that in general networks, the SD is proportional to $N^{1/2}$ for small N but converges to a finite value for large N; there is a crossover. Based on our results, design principle of precise biological pacemaker is discussed.

(S12 – T5) Co-evolutionary networks as a model for genetic regulation

K. Bassler

Physics Department, University of Houston, Texas, USA

(S12 – P1) Statistical description of subgraph fluctuations in random graphs

Christoph Fretter[1], *Matthias Müller-Hannemann*[1] *and Marc-Thorsten Hütt*[2]

[1]Institut für Informatik, Martin-Luther Universität Halle-Wittenberg, Germany

[2]School of Engineering and Science, Jacobs University, Bremen, Germany

The pattern of over- and under-representations of three-node subgraphs has become a standard method of characterizing complex networks and evaluating, how this intermediate level of organization contributes to network function. We explored this relationship in previous publications [1,2]. Understanding statistical properties of subgraph counts in random graphs, their fluctuations and their interdependencies with other topological attributes is an important prerequisite for such investigations [3]. Here we introduce a formalism for predicting subgraph fluctuations induced by perturbations of uni-directional and bi-directional edge densities. On this basis we predict the over- and under-representation of subgraphs arising from a density mismatch between a network and the corresponding pool of randomized graphs serving as null model. Such mismatches occur for example in modular and hierarchical graphs.

[1] Krumov L., Fretter, C., Müller-Hannemann, M., Weihe, K. and Hütt, M.-Th., Motifs in co-authorship networks and their relation to the impact of scientific publications. *Eur. Phys. J. B,* (2011) in press.

[2] Marr, C., Theis, F.J., Liebovitch, L.S. and Hütt, M.-Th., Patterns of subnet usage in the transcriptional regulatory network of Escherichia coli. *PLoS Computational Biology* **6**, e1000836 (2010).

[3] Fretter, C., Beber, M., Müller-Hannemann, M. and Hütt, M.-Th., Artifacts in statistical analyses of network motifs. *J. R. Soc. Interface*, (2011) submitted.

(S12 – P2) Design of robust flow processing networks with time-programmed responses

Pablo Kaluza, Alexander Mikhailov
Department of Physical Chemistry, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

We design flow-processing networks with time-programmed responses. This network model allows us to consider situations when activation of an input node triggers a coordinated series of responses in different output nodes, generating a specific temporal pattern. A network is not only designed to be functional performing a target response, it is also optimized to be robust against local damages as the deletion of one its nodes or one of its links. We show that the design of robust functional networks is possible by applying evolutionary optimization algorithms of mutations and selections. We present the main properties of these networks, including their motif distributions, as function of the different robust design criteria. Finally, we present the case of steady flows for this model and its relationship with previously considered static flow distribution network model [1,2].

[1] Kaluza, P., M. Ipsen, M. Vingron, and A. S. Mikhailov. Design and statistical properties of robust functional networks: A model study of biological signal transduction. *Phys. Rev. E.*, **75**, 015101 (2007).
[2] Kaluza, P., M. Vingron, and A. S. Mikhailov. Self-correcting networks: Function, robustness, and motif distributions in biological signal processing. *Chaos,* **18**, 026113 (2008).

(S12 – P3) On distance-based graph entropies

Lavanya Sivakumar, Matthias Dehmer
Institute of Bioinformatics and Translational Research, UMIT, 6060 Hall, Austria

Entropy-based descriptors have been widely used to quantify structural information of networks [1,2]. In this talk, we put the emphasis on distance-based graph entropies. Note that various information-theoretic network measures based on the so-called distance code, the distance-degree sequence, and certain graph-theoretical matrices have been developed [3]. However, the usefulness of many of these measures has never been demonstrated and, moreover, some of these measures lack a clear graph-theoretical interpretation. Consequently, we report some interesting properties thereof such as discrimination power, similarity and correlations and point out further advantages and disadvantages of this particular class of graph entropies when being applied to large scale complex networks.

[1] D. Bonchev, *Information Theoretic Indices for Characterization of Chemical Structures*. (Research Studies Press, Chichester 1983).
[2] M. Dehmer, Information processing in complex networks: Graph entropy and information functionals. *Appl. Math. Comput.*, **201,** 82–94 (2008).
[3] R. Todeschini and V. Consonni, *Molecular Descriptors for Chemoinformatics: Alphabetical Listing*, volume 1&2. (Wiley-VCH, 2nd edition, 2009).

(S12 – P4) A new approach to comparison of two graphs

Olga Valba [1,2], *S.K. Nechaev* [2], *M.V. Tamm* [3]
[1] Moscow Institute of Physics and Technology, Dolgoprudny, Russia, [2] LPTMS, University Paris Sud, Orsay, France, [3]Physics Department, Moscow State University, Moscow, Russia

Comparison of two graphs or the maximum common subgraph problem has important practical applications in many areas of bioinformatics as well as in other areas, such as pattern recognition and image processing. The problem belongs to NP complexity class, however more and more new methods are developed nowadays [1]. We propose a new method of finding the largest common subgraph of two graphs, which is based on "correct" numbering of the vertices in the comparable graphs. This "correct" numeration allows to write graphs in unique arc diagram representation and effectively determine their maximum common part. We have applied our method to real biological networks and model random graphs. Also, the proposed procedure can be used for finding of cliques and strong connected components in a graph. We present some results for random hierarchical networks.

[1] Roded Sharan and Trey Ideker, Modelling cellular machinery through biological network comparison, *Nature Biotechnology,* **24**, 427-433 (2006).

Symposium 13: **Mathematical Aspects**

(S13 – T1) Waves in heterogeneous media and their application to adaptive behavior of *Physarum plasmodium*

Yasumasa Nishiura[1], *Kei-Ichi Ueda*[2], *Seiji Takagi*[1], *Toshi Nakagaki*[3]
[1] Research Institute for Electronic Science, Hokkaido University, Sapporo, [2] Department of Mathematics, Toyama University, [3] Department of Complex and Intelligent Systems, Future University Hakodate

It has recently been reported that even single-celled organisms appear to be “indecisive” or “contemplative” when confronted with an obstacle. When the amoeboid organism *Physarum* plasmodium encounters the chemical repellent quinine during migration along a narrow agar lane, it stops for a period of time (typically several hours) and then suddenly begins to move again. When movement resumes, three distinct types of behavior are observed: The plasmodium continues forward, turns back, or migrates in both directions simultaneously. Here we develop a continuum mathematical model of the cell dynamics of contemplative amoeboid movement. Our model incorporates the dynamics of the mass flow of the protoplasmic sol, in relation to the generation of pressure based on the autocatalytic kinetics of pseudopod formation and retraction (mainly, sol-gel conversion accompanying actin-myosin dynamics).

[1] K.-I.Ueda, S.Takagi, Y.Nishiura and T.Nakagaki, Mathematical model for contemplative amoeboid locomotion. *Phys. Rev. E,* **83**, 021916 (2011).

(S13 – T2) Coarse-graining dynamics on the networks, and of the networks

Ioannis Kevrekidis
Dept. of Chemical Engineering and Engineering Quadrangle,
Princeton University, Princeton, NJ, USA

(S13 – T3) Structure of regulatory networks and dynamics of bio-molecules: Predicting unknown from known

Atsushi Mochizuki[1], *Bernold Fiedler*[2], *Daisuke Saito*[1]
[1] RIKEN Advanced Science Institute, Japan, [2] Department of Mathematics, Free University of Berlin, Germany

Regulatory relations between biological molecules constitute complex network systems, and realize diverse biological functions through the dynamics of molecular activities. In this study we introduce a new method, named “linkage logic”, to analyze the dynamics of network systems. By this method, we can restrict possible dynamical behaviors of a given complex network system from the knowledge of regulatory linkages alone. Applications of the methods are the followings: (i) for a given network, we can identify a cluster of nodes that gives an alternative representation of the attractors of the whole system, (ii) we can reduce a given complex network into a simpler one without loss of the ability to generate the diversity of solutions, (iii) we can examine the consistency between the structure of network and observed set of steady states, and (iv) sometimes we can predict unknown states or unknown regulations from an observed set of steady states alone. We illustrate the method by several applications to an experimentally determined regulatory network for biological functions.

[1] Mochizuki A. and Saito D., Analyzing steady states of dynamics of biomolecules from the structure of regulatory networks *J. Theor. Biol.,* **266**, 323-335 (2010).

[2] Fiedler B. and Mochizuki A. (In preparation).

(S13 – T4) Identification of gene regulatory cycles: Theory and applications

B. Fiedler
Department of Mathematics, Free University of Berlin, Germany

(S13 – P1) Feedback control of nonlinear dissipative systems: A reaction-diffusion paradigm

Abderrahim Azouani
Department of Mathematics, Free University of Berlin, Germany

List of Participants

1. Prof. Mazen Al-Ghoul (S01 – P1), Dept. of Chemistry, American University of Beirut, mazen.ghoul@aub.edu.lb

2. Dr. Sergio Alonso (S06 – T2), Physikalisch-Technische Bundesanstalt (PTB), Berlin, Sergio.Alonso@ptb.de

3. Mr. Adithya Ananth (S09 – P1), Leibniz Institute for Solid State and Materials Research (IFW), Dresden, a.n.ananth@ifw-dresden.de

4. Dr. Arash Azhand (S01 – P2), Dept. of Physics, Technical University of Berlin, azhand@itp.tu-berlin.de

5. Dr. Abderrahim Azouani (S13 – P1), Dept. of Mathematics, Free University of Berlin, azouani@hotmail.com

6. Prof. Markus Bär (S06), Physikalisch-Technische Bundesanstalt (PTB), Berlin, Markus.Baer@ptb.de

7. Prof. Takahiko Ban (S06 – P1), Dept. of Chemical Engineering and Materials Science, Doshisha University, Kyoto, tban@mail.doshisha.ac.jp

8. Dr. Larysa Baraban, Leibniz Institute for Solid State and Materials Research (IFW), Dresden, l.baraban@ifw-dresden.de

9. Ms. Eva Baresel (S09 – P2), Dept. of Physics, Westf. Wilhelms University, Münster, eva.baresel@uni-muenster.de

10. Prof. Kevin E. Bassler (S12 – T5), Physics Dept., University of Houston, Texas, bassler@uh.edu

11. Mr. Philipp Bauer (S07 – P1), Dept. of Physics, Technical University of München, pbauer@ph.tum

12. Dr. Igal Berenstein (S01 – P3), Institute for Physics and Astronomy, University of Potsdam, berenst@uni-potsdam.de

13. Ms. Adriana Bernal Osorio (S07 – T3), Dept. of Physical Chemistry, Fritz Haber Institute of the Max Planck Society, Berlin, adbeos@fhi-berlin.mpg.de

14. Dr. Helene Berthoumieux (S10 – P1), Max Planck Institute for Physics of Complex Systems, Dresden, bhelene@pks.mpg.de

15. Prof. Carsten Beta, Institute of Physics and Astronomy, University of Potsdam, carsten.beta@uni-potsdam.de

16. Prof. Adrian Birzu (S07 – P2) and (S08 – P1), Faculty of Chemistry, Al. I. Cuza University, Iasi, abirzu@uaic.ro

17. Prof. Eberhard Bodenschatz (S08), Max Planck Institute for Dynamics and Self-Organization, Göttingen, eberhard.bodenschatz@ds.mpg.de

18. Ms. Astrid Lilian Bornhöft, Dept. of Physics, Otto von Guericke University, Magdeburg, astrid.bornhoeft@ovgu.de

19. Prof. Stefan Bornholdt (S12 – T1), Dept. of Physics, University of Bremen, bornholdt@itp.uni-bremen.de

20. Mr. Rico Buchholz (S01 – P2), Dept. of Physics, Technical University of Berlin, rico.buchholz@physik.tu-berlin.de

21. Dr. Marcello Budroni (S03 – P1), University of Siena, Italy, mabudroni@uniss.it

22. Mr. Domenico Bullara (S01 – P4), Nonlinear Physical Chemistry Unit, Université Libre de Bruxelles, Bruxelles, dbullara@ulb.ac.be

23. Ms. Natalie Busch, Dept. of Physics, Technical University of Berlin; natalie@itp.tu-berlin.de

24. Mr. Jorge Carballido-Landeira (S08 – P2), Group of Nonlinear Physics, Universidad de Santiago de Compostela, jorge.carballido@gmail.com

25. Dr. Hugues Chaté (S06 – T3), Service de Physique de l'Etat Condensé, CEA Saclay, hugues.chate@cea.fr

26. Dr. Markus A. Dahlem (S08 – T2), Dept. of Physics, Technical University of Berlin, dahlem@physik.tu-berlin.de

27. Dr. Yves Dauphin, Innovation Centre, SOLVAY S.A., Brussels, Yves.Dauphin@solvay.com

28. Prof. Joern Davidsen (S12 – T2), Complexity Science Group, University of Calgary, joern.davidsen@ucalgary.ca

29. Dr. Pierre de Buyl (S09 – P3), Chemistry Dept., University of Toronto, pdebuyl@chem.utoronto.ca

30. Prof. Matthias Dehmer, Institute for Bioinformatics and Translational Research, UMIT, Hall in Tyrol, Austria, Matthias.Dehmer@umit.at

31. Dr. Yves Dehouck (S10 – P2), Dept. of Physical Chemistry, Fritz Haber Institute of the Max Planck Society, Berlin, ydehouck@fhi- berlin.mpg.de

32. Mr. Markus Düttmann (S10 – P3), Dept. of Physical Chemistry, Fritz Haber Institute of the Max Planck Society, Berlin, duettmann@fhi-berlin.mpg.de

33. Mr. Piotr Dziekan (S11 – P1), Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw, pdziekan@ichf.edu.pl

34. Prof. Werner Ebeling, Institute of Physics, Humboldt University of Berlin, ebeling@physik.hu-berlin.de

35. Dr. Blas Echebarria (S01 – T4), Departament Física Aplicada, Universitat Politècnica de Catalunya, Barcelona, blas@.upc.edu

36. Prof. Manfred Eigen (P1), Max Planck Institute for Biophysical Chemistry, Göttingen

37. Dr. Mihaela Enculescu (S10– T4) & (S09 – P4), Dept. of Physics, Technical University of Berlin, mihaela.enculescu@tu-berlin.de

38. Prof. Harald Engel (S01 – I), Dept. of Physics, Technical University of Berlin, h.engel@physik.tu-berlin.de

39. Prof. Irving R. Epstein (S02 – I), Dept. of Chemistry, Brandeis University, USA, epstein@brandeis.edu

40. Prof. Gerhard Ertl, Dept. of Physical Chemistry, Fritz Haber Institute of the Max Planck Society, Berlin, ertl@fhi-berlin.mpg.de

41. Dr. Martin Falcke (S10 – I), Max Delbrück Center for Molecular Medicine, Berlin, martin.falcke@mdc-berlin.de

42. Prof. Vera Maura Fernandes de Lima, Biotechnology Centre, Nuclear Energy Research Institute (IPEN/CNEN/SP), São Paulo, Brazil, vmflima@ipen.br

43. Prof. Bernold Fiedler (S13 – T4), Dept. of Mathematics, Free University of Berlin, fiedler@math.fu-berlin.de

44. Mr. Holger Flechsig (S10 – P5), Dept. of Physical Chemistry, Fritz Haber Institute of the Max Planck Society, Berlin, flechsig@fhi-berlin.mpg.de

45. Mr. Christoph Fretter (S12 – P1), Institute for Informatics, Martin Luther University of Halle-Wittenberg~~,~~ christoph.fretter@gmx.de

46. Mr. Stefan Fruhner (S01 – P5), Dept. of Physics, Technical University of Berlin, stefan.fruhner@tu-berlin.de

47. Dr. Simon Fugmann, Dept. of Physics, Humboldt University of Berlin, simon.fugmann@physik.hu-berlin.de

48. Dr. Naoya Fujiwara (S03 – P2), Potsdam Institute for Climate Impact Research, fujiwara@pik-potsdam.de

49. Dr. Qingyu Gao (S08 – P3), School of Chemistry and Engineering, China University of Mining and Technology, Xuzhou, Gaoqy@cumt.edu.cn

50. Dr. Vladimir Garcia-Morales (S11 – T2), Dept. of Physics, Technical University of München, vmorales@ph.tum.de

51. Prof. Pierre Gaspard (P3), Dept. of Physics, Université Libre de Bruxelles, gaspard@ulb.ac.be

52. Dr. Dan T. Gillespie (S11 – T1), Dan T Gillespie Consulting, USA, gillespiedt@mailaps.org

53. Ms. Miriam Grace (S10 – P6), Dept. of Physics, Jacobs University Bremen, m.grace@jacobs-university.de

54. Dr. Leonhard Grill (S04 – I), Dept. of Physical Chemistry, Fritz Haber Institute of the Max Planck Society, Berlin, lgr@fhi-berlin.mpg.de

55. Dr. Stephan Grill (S10 – T3), Max Planck Institute for Physics of Complex Chemical Systems and Max Planck Institute for Molecular Cell Biology and Genetics, Dresden, grill@mpi-cbg.de

56. Dr. Thilo Gross (S12 – T1), Max Planck Institute for Physics of Complex Chemical Systems, Dresden, thilo.gross@physics.org

57. Mr. Robert Großmann, Dept. of Physics, Humboldt University of Berlin, grossmann@physik.hu-berlin.de

58. Dr. Svetlana Gurevich (S08 – T4), Institute for Theoretical Physics, University of Münster, gurevics@uni-muenster.de

59. Dr. Richard Hanke-Rauschenberg, Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg, hanke-rauschenbach@mpi-magdeburg.mpg.de

60. Mr. Shigefumi Hata (S03 – P3), Dept. of Physics, Kyoto University, hata@ton.scphys.kyoto-u.ac.jp

61. Prof. Marcus Hauser (S01 – P6), Dept. of Physics, Otto von Guericke University, Magdeburg, marcus.hauser@physik.uni-magdeburg.de

62. Mr. Robert Hölzel, Dept. of Physics, Technical University of München, rhoelzel@ph.tum.de

63. Dr. Marcel Hörning (S08 – P4), Kyoto University, marcel@chem.scphys.kyoto-u.ac.jp

64. Dr. Judit Horváth (S02 – T2), Institute of Chemistry, Eötvös Loránd University, Budapest, holmes@chem.elte.hu

65. Prof. Zhonghuai Hou (S11 – T4), Dept. of Chemical Physics, University of Science and Technoloy of China, Hefei, hzhlj@ustc.edu.cn

66. Mr. Mu-Jie Huang (S06 – P2), Dept, of Biophysics, National Central University, Jhongli, Taiwan, jthebes@gmail.com

67. Prof. John L. Hudson (S07), Dept. of Chemical Engineering, University of Virginia, Charlottesville, hudson@virginia.edu

68. Dr. Masatoshi Ichikawa (S06 – P3), Dept. of Physics, Kyoto University, ichi@scphys.kyoto-u.ac.jp

69. Prof. Ronald Imbihl, Institute for Physical Chemistry and Electrochemistry, Leibniz University, Hannover, imbihl@pci.uni-hannover.de

70. Dr. Masayo Inoue (S10 – P7), Cybermedia Center, Osaka University, inoue@cp.cmc.osaka-u.ac.jp

71. Mr. Thomas M. Isele (S01 – P7), Dept. of Physics, Technical University of Berlin, tommaso@itp.tu-berlin.de

72. Dr. Pablo Kaluza (S12 – P2), Dept. of Physical Chemistry, Fritz Haber Institute of the Max Planck Society, Berlin, kaluza@fhi-berlin.mpg.de

73. Dr. Atsushi Kamimura (S05 – T3) and (S11 – T5), Institute of Industrial Science, University of Tokyo, kamimura@sat.t.u-tokyo.ac.jp

74. Prof. Kunihiko Kaneko (S05 – T2 & P1), Dept. of Basic Science and Research Center for Complex Systems Biology, University of Tokyo, kaneko@complex.c.u-tokyo.ac.jp

75. Prof. Raymond E. Kapral (P5), Dept. of Chemistry, University of Toronto, rkapral@chem.utoronto.ca

76. Prof. Ioannis G. Kevrekidis (S13 – T2), Dept. of Chemical Engineering and Engineering, Princeton University, yannis@arnold.princeton.edu

77. Mr. Sebastian Kirsch, Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg, kirsch@mpi-mpg.de

78. Prof. Istvan Z. Kiss (S03 – T2), Dept. of Chemistry, Saint Louis University, USA, izkiss@slu.edu

79. Mr. Peter E. Klages (S07 – T4), Dept. of Physics and Atmospheric Science, Dalhousie University, Halifax, Canada, pklages@dal.ca

80. Dr. Tetsuya J. Kobayashi (S11-T3), Institute of Industrial Science, University of Tokyo, tetsuya@mail.crmind.net

81. Mr. Marek Kolmer (S04 – P2), Institute of Physics, Jagiellonian University, Kraków, marek.kolmer@gmail.com

82. Prof. Hiroshi Kori (S12 – T4), Ochanomizu University, Tokyo, kori.hiroshi@ocha.ac.jp

83. Dr. Aneta Koseska (S03 – T3), Interdisciplinary Center for Dynamics of Complex Systems, University of Potsdam, koseska@yahoo.com

84. Dr. Nikos Kouvaris (S03 –P4), Dept. of Physical Chemistry, Fritz Haber Institute of the Max Planck Society, Berlin, nkoub@chem.demokritos.gr

85. Prof. Katharina Krischer (S07 – I), Dept. of Physics, Technical University of München, krischer@ph.tum.de

86. Prof. Karsten Kruse (S01 – T3), Dept. of Physics, University of Saarland, Saarbrücken, k.kruse@physik.uni-saarland.de

87. Dr. Takashi Kumagai (S04 – P1), Dept. of Physical Chemistry, Fritz Haber Institute of the Max Planck Society, Berlin, kuma@fhi-berlin.mpg.de

88. Mr. Dennis Kupitz (S01 – P8), Dept. of Physics, Otto von Guericke University, Magdeburg, dennis.kupitz@st.ovgu.de

89. Prof. Krisztina Kurin-Csörgei (S03 – P5), Dept. of Inorganic and Analytical Chemistry, Eötvös University, Budapest, kurin@chem.elte.hu

90. Prof. Jürgen Kurths (S03 –I), Potsdam Institute for Climate Impact Research, juergen.kurths@pik-potsdam.de

91. Mr. Luis F. Lafuerza (S11 – P2), IFISC (UIB-CSIC), Palma de Mallorca, Spain, luis@ifisc.uib-csic.es

92. Prof. István Lagzi (S03 – T5), Dept. of Theoretical Physics, Eötvös University, Budapest, lagzi@vuk.chem.elte.hu

93. Dr. David Laroze (S08 – T5), Max Planck Institute for Polymer Research, Mainz, david.laroze@gmail.com

94. Dr. Annie Lemarchand (S11 – P3), Lab. de Physique Théorique de la Matière Condensée, Université Pierre et Marie Curie – CNRS, Paris, anle@lptmc.jussieu.fr

95. Ms. Claudia Lenk (S03 – T4), Institute for Physics, Technical University of Ilmenau, claudia.lenk@tu-ilmenau.de

96. Prof. Albert Libchaber (S05 – T1), The Rockefeller University, New York, libchbr@rockefeller.edu

97. Prof. Katja Lindenberg (S11 – I), Dept. of Chemistry and Biochemistry, University of California San Diego, La Jolla, klindenberg@ucsd.edu

98. Prof. Trolle R. Linderoth (S04 – T2), Dept. of Physics and Astronomy, Aarhus University, Denmark, trolle@inano.dk

99. Dr. Haimiao Liu (S08 – P3), College of Chemical Engineering, China University of Mining & Technology, Xuzhou, liuhaimiao0814@163.com

100. Mr. Jakob Löber (S01 – P9), Dept. of Physics, Technical University of Berlin, jakob@physik.tu-berlin.de

101. Prof. Stefan Luther (S08 – T3), Max Planck Institute for Dynamics and Self-Organization, Göttingen, stefan.luther@ds.mpg.de

102. Dr. Susanna C. Manrubia (S05 – I), Centro de Astrobiología, INTA-CSIC, Madrid, scmanarubia@cab.inta.csic.es

103. Mr. Martin Marmulla (S01 – P9), Dept. of Physics, Technical University of Berlin, marmulla@itp.tu-berlin.de

104. Mr. Steffen Martens, Dept. of Physics, Humboldt University of Berlin, steffen.martens@physik.hu-berlin.de

105. Dr. Gerhard Meyer (S04 – T1), IBM Research Zurich, gme@zurich.ibm.com

106. Prof. Alexander S. Mikhailov, Dept. of Physical Chemistry, Fritz Haber Institute of the Max Planck Society, Berlin, mikhailov@fhi-berlin.mpg.de

107. Dr. Atsushi Mochizuki (S13 – T3), RIKEN Advanced Science Institute, Wako, Japan, mochi@riken.jp

108. Ms. Sonja Molnos, Dept. of Physics, Technical University of Berlin, sonja@molnos.de

109. Dr. Fumito Mori (S03 – P6), Ochanomizu University, Tokyo, mori.fumito@ocha.ac.jp

110. Ms. Andressa Mota (S07 – P3), Dept. of Physical Chemistry, Fritz Haber Institute of the Max Planck Society, Berlin, mota@fhi-berlin.mpg.de

111. Dr. Stefan Müllegger (S04 – T3), Solid State Physics, Johannes Kepler University, Linz, Austria, stefan.muellegger@jku.at

112. Prof. Stefan C. Müller, Dept. of Physics, Otto von Guericke University, Magdeburg, stefan.mueller@physik.uni-magdeburg.de

113. Prof. Alberto P. Muñuzuri (S01 – P10), Nonlinear Physics, Universidad de Santiago de Compostela, Spain, alberto.perez.munuzuri@usc.es

114. Mr. Frantisek Muzika (S08 – P5), Dept. of Chemical Engineering, Institute of Chemical Technology, Prague, frantisek.muzika@vscht.cz

115. Prof. Yuichiro Nagatsu (S06 – P4), Dept. of Materials Science and Engineering, Nagoya Institute of Technology, nagatsu@nitech.ac.jp

116. Mr. Robert Niedl (S01 – P11), Institute of Physics and Astronomy, University of Potsdam, niedl@uni-potsdam.de

117. Dr. Masatoshi Nishikawa (S10 – P8), Labs for Physical Biology, RIKEN Center for Developmental Biology, Kobe, masnishi@cdb.riken.jp

118. Prof. Yasumasa Nishiura (S13 – T1), Research Institute for Electronic Science, Hokkaido University, Sapporo, nishiura@aurora.es.hokudai.ac.jp

119. Dr. Katarina Novakovic (S03 – P7), School of Chemical Engineering, Newcastle University, UK, katarina.novakovic@ncl.ac.uk

120. Dr. Bogdan Nowakowski (S11 – P1), Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw, bnowakowski@ichf.edu.pl

121. Prof. Takao Ohta (S06 – I), Dept. of Physics, Kyoto University, takao@scphys.kyoto-u.ac.jp

122. Prof. Miklós Orbán (S03 – P5), Dept. of Inorganic and Analytical Chemistry, Eötvös University, Budapest,

orbanm@chem.elte.hu

123. Mr. Fabian Paul (S01 – P12), Dept. of Physics, Technical University of Berlin, fab@physik.tu-berlin.de

124. Dr. Fernando Peruani (S09 – T6), Max Planck Institute for Physics of Complex Systems, Dresden, peruani@pks.mpg.de

125. Prof. Peter Plath, Dept. of Physical Chemistry, Fritz Haber Institute of the Max Planck Society, Berlin, plath@fhi-berlin.mpg.de

126. Prof. Harald Pleiner, Max Planck Institute for Polymer Research, Mainz, pleiner@mpip-mainz.mpg.de

127. Dr. Jakub Prauzner-Bechcicki (S04 – P2), Institute of Physics, Jagiellonian University, Kraków, bechcicki@uj.edu.pl

128. Prof. Qi Ouyang (P4), Center for Theoretical Biology, Peking University, Beijing, qi@pku.edu.cn

129. Mr. Markus Radszuweit (S02 – P1), Dept. of Physics, Technical University of Berlin, radszuweit@itp.tu-berlin.de and PTB Berlin, Markus.Radszuweit@ptb.de

130. Ms. Elizeth Ramirez-Alvarez (S07 – P4), Instituto Tecnológico de Celaya, México, elizethra@yahoo.com

131. Ms. Teresa E. Reinhard, Dept. of Physics, Technical University of Berlin, teresa.e.reinhard@campus.tu-berlin.de

132. Dr. Pawel Romanczuk (S09 – T5), Max Planck Institute for Physics of Complex Systems, Dresden, prom@pks.mpg.de

133. Dr. Diana I. Roncaglia (S01 – P13), D.to de Ciencia y Tecnología, Universidad Nacional de Quilmes, Buenos Aires, diana@unq.edu.ar

134. Dr. Federico Rossi (S03 – P8), Ecodynamics Group, University of Siena, Italy, f.rossi@unisi.it

135. Prof. Harm H. Rotermund (S07), Dept. of Physics and Atmospheric Science, Dalhousie University, Halifax, Canada, harm.rotermund@dal.ca

136. Dr. Sten Rüdiger (S10 – P9), Dept. of Physics, Humboldt University Berlin, sten.ruediger.gmail.com

137. Mr. Benedikt Sabass (S09 – P4), II Institute for Theoretical Physics, Stuttgart University, sabass@theo2.physik.uni-stuttgart.de

138. Prof. Francesc Sagués (S09 – T3), Departament de Química Física, Universitat de Barcelona, f.sagues@ub.es

139. Prof. Dominique Salin (S03 – P9), Université Pierre et Marie Curie, Orsay, dominique.salin@upmc.fr

140. Dr. Samuel Sanchez (S09 – P5), Leibniz Inst. for Integrative Nanosciences, IWF Dresden, s.sanchez@ifw-dresden.de

141. Prof. Satoshi Sawai (S10 – T1), University of Tokyo, cssawai@mail.ecc.u-tokyo.ac.jp

142. Prof. Lutz Schimansky-Geier (S09 – I), Dept. of Physics, Humboldt University of Berlin, alsg@physik.hu-berlin.de

143. Prof. Eckehard Schöll (S08 – I), Dept. of Physics, Technical University of Berlin, schoell@physik.tu-berlin.de

144. Prof. Igor Schreiber, Dept. of Chemical Engineering, Inst. of Chemical Technology, Prague, Igor.Schreiber@vscht.cz

145. Dr. Hanna Sciegosz, Faculty of Management, Opole University of Technology, Poland, sciegosz@po.opole.pl

146. Dr. Gabriel Seiden (S08 – T1), Physics of Complex Systems, Weizmann Institute of Science, Israel, gabriel.seiden@weizmann.ac.il

147. Prof. Ayusman Sen (S09 – T1), Dept. of Chemistry, Pennsylvania State University, asen@psu.edu

148. Dr. M. Angeles Serrano (S12 – T3), Departament de Química Física, Universitat de Barcelona, marian.serrano@ub.edu

149. Dr. Tatsuo Shibata (S10 – T2), RIKEN Center for Developmental Biology, Kobe, tatsuoshibata@cdb.riken.jp

150. Prof. Kenneth C. Showalter (S09 – T2), Dept. of Chemistry, West Virginia University, USA, kshowalt@wvu.edu

151. Dr. Lavanya Sivakumar (S12 – P3), UMIT, Hall in Tirol, Austria, lavanya.sivakumar@umit.at

152. Prof. Igor Sokolov (S11 – I), Dept. of Physics, Humboldt University of Berlin, igor.sokolov@physik.hu-berlin.de

153. Prof. Holger Stark (S01 – T2), Dept. of Physics, Technical University of Berlin, Holger.Stark@tu-berlin.de

154. Prof. Oliver Steinbock (S01 – T1), Dept. of Chemistry and Biochemistry, Florida State University, Tallahassee, steinbck@chem.fsu.edu

155. Prof. Tadashi Sugawara (S06 – T1), Graduate School of Arts and Sciences, University of Tokyo, suga@pentacle.c.u-tokyo.ac.jp

156. Prof. Kai Sundmacher (S07 – T1), Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg, sundmacher@mpi-magdeburg.mpg.de

157. Prof. István Szalai (S01 – P14), Institute of Chemistry, Eötvös University, Budapest, pisti@chem.elte.hu

158. Mr. Jan Szymanski (S01 – P15), Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw, jszymanski@ichf.edu.pl

159. Mr. Fumi Takabatake (S06 – P5), Dept. of Physics, Kyoto University, takabatake@chem.scphys.kyoto-u.ac.jp

160. Mr. Nándor Takács (S01 – P16), Institute of Chemistry, Eötvös Loránd University, Budapest, tnandi@caesar.elte.hu

161. Dr. Kazumasa Takeuchi (S07 – T2), University of Tokyo / SPEC, CEA-Saclay, kazumasa@daisy.phys.s.u-tokyo.ac.jp

162. Dr. Xiaodong Tang (S01 – P17), School of Chemistry and School of Chemistry and Engineering, China University of Mining and Technology, Xuzhou, windmillons@126.com

163. Mr. Mitsusuke Tarama (S09 – P6), Dept. of Physics, Kyoto University, tarama@ton.scphys.kyoto-u.ac.jp

164. Dr. Annette F. Taylor (S03 – T1), School of Chemistry, University of Leeds, A.F.Taylor@leeds.ac.uk

165. Mr. Shashi Thutupalli (S06 – T4), Max Planck Institute for Dynamics and Self-Organization, Göttingen, ashi.thutupalli@ds.mpg.de

166. Dr. Ralf Toenjes (S03 – P10), Ochanomizu University, Tokyo, rahleph@gmail.com

167. Mr. Yousuke Tonosaki (S08 – P6), Dept. of Physics, Kyoto University, Kyoto, tonosaki@ton.scphys.kyoto-u.ac.jp

168. Ms. Olga Valba (S12 – P4), LPTMS, Centre Scientifique d'Orsay, Université Paris Sud, Orsay, olga.valba@lptms.u-psud.fr

169. Dr. Daniel Weise (S01 – P18), Theoretical Biology, Utrecht University, weises-daniel@gmx.de

170. Ms. Magdalena Wrobel (S03 – P11), School of Chemistry, University of Leeds, cmmmw@leeds.ac.uk

171. Dr. Wang Xi, Leibniz Institute for Solid State and Materials Research (IFW), Dresden, w.xi@ifw-dresden.de

172. Prof. Bing Xu (S02 – T3), Dept. of Chemistry, Brandeis University, USA, bxu@brandeis.edu

173. Prof. Toshio Yanagida (P2), Labs for Nanobiology (Soft Biosystem Group), Graduate School of Frontier Biosciences, Osaka University, yanagida@phys1.med.osaka-u.ac.jp

174. Dr. Victor Yashin (S02 – T4), Chemical Engineering Dept., University of Pittsburgh, USA, vvy1@pitt.edu

175. Prof. Ryo Yoshida (S02 – T1), Dept. of Materials Engineering, University of Tokyo, ryo@cross.t.u-tokyo.ac.jp