CeCAM Workshop - Abstracts





Charged Species in Bulk and Interfaces: Mobility and Motility of Macromolecular Systems

September 24-27, 2018

TU Wien Campus Gußhaus, Lecture Hall EI 10 "Fritz Paschke" 1040 Vienna, Gußhausstraße 27-29

Organizers: Kyongok Kang, Forschungszentrum Jülich, Germany Gerhard Kahl, TU Wien, Austria Jan Dhont, Forschungszentrum Jülich, Germany

Charged Species in Bulk and Interfaces: Mobility and Motility of Macromolecular Systems

September 24-27, 2018, TU Wien

13:30 - 14:30	Welcoming Reception & Registration
14:30 - 15:00	Introduction of Workshop by Organizers Kyongok Kang, Gerhard Kahl, and Jan Dhont *** Reflection on our last Workshop & estimation of this one
15:00 - 15:40	Gerhard Nägele (ICS-3, Forschungszentrum Jülich, Germany)
15:40 - 16:20	Akira Onuki (Kyoto University, Japan)
16:20 - 16:50	Tea/Coffee Break
16:50 - 17:30	Jure Dobnikar (Univ. of Cambridge, UK, Chinese Acad. of Sciences, China)
19:00 - 21:00	Workshop Dinner - Let's be together!

Day 1 - September 24, 2018

Day 2 - September 25, 2018

08:40 - 09:00	Registration of Day 2
09:00 - 09:40	Alan Denton (North Dakota State University, USA)
09:40 - 10:20	Jan-Philip Machtens (ICS-4, Forschungszentrum Jülich, Germany)
10:20 - 10:50	Tea/Coffee Break
10:50 - 11:30	Jérome Crassous (Lund University, Sweden / RWTH Aachen, Germany)
11:30 - 12:10	Christos N. Likos (University of Vienna, Austria)
12:10 - 13:40	Lunch Break
13:40 - 14:20	Malin Zackrisson Oskolkova (Novo Nordisk A/S, Denmark)
14:20 - 15:00	Roland R. Netz (Free Univ. of Berlin, Germany)
15:00 - 15:30	Tea/Coffee Break
15:30 - 16:10	Alexey Eremin (University of Magdeburg, Germany)
16:10 - 16:50	Frank Schreiber (University of Tübingen, Germany)
16:50 - 17:30	Peter Fischer (D-HEST, ETHZ, Zurich, Switzerland)
17:30 - 19:00	Open Discussion: Day 2

08:40 - 09:00	Registration of Day 3
09:00 - 09:40	Orlin D. Velev (North Carolina State University, USA)
09:40 - 10:20	Jens Harting (Helmholtz Institute Erlangen-Nürnberg, Forschungszentrum Jülich, Germany)
10:20 - 10:50	Tea/Coffee Break
10:50 - 11:30	Emmanuel Trizac (Université Paris-Sud, France)
11:30 - 12:10	Ben Werkhoven (Utrecht University, The Netherlands)
12:10 - 13:40	Lunch Break
13:40 - 14:20	Filip Strubbe (Ghent University, Belgium)
14:20 - 15:00	Vania Calandrini (INM-9 & IAS-5, Forschungszentrum Jülich, Germany)
15:00 - 15:30	Tea/Coffee Break
15:30 - 16:10	Paolo Carloni (INM-9 & IAS-5, Forschungszentrum Jülich, Germany)
16:10 - 16:50	Emanuela Bianchi (University of Vienna / TU Wien, Austria)
16:50 - 17:30	Clemens Jochum (TU Wien, Austria)
17:30 - 19:00	Open Discussion: Day 3

Day 3 - September 26, 2018

Day 4 - September 27, 2018

08:40 - 09:00	Registration of Day 4
09:00 - 09:40	Daniel Hammer (University of Pennsylvania, USA)
09:40 - 10:20	Christoph Goegelein (LANXESS GmbH, Germany)
10:20 - 10:50	Tea/Coffee Break
10:50 - 11:30	Anselm Horn (Friedrich-Alexander-Univ., Erlangen-Nürnberg, Germany)
11:30 - 11:45	Summary of Workshop (by Jan Dhont)
11:45 - 12:00	Closing Remarks of Workshop & Feedback

Charged Species in Bulk and Interfaces: Mobility and Motility of Macromolecular Systems

September 24-27, 2018, TU Wien

Abstracts

Monday, September 24, 2018

15:00 - 15:40	Gerhard Nägele (ICS-3, Forschungszentrum Jülich, Germany)	
Diffusion and	dynamic scaling in charge - stabilized colloidal suspensions	
Dispersions of Brownian particles interacting by a screened Coulomb pair potential are a paradigm for a variety of charge - stabilized colloidal suspensions and globular protein solutions encountered in chemical industry, biology and medicine.		
I report on a c diffusion in sus spheres interact intermediate sc where hydrody short - time to mode - coupling enhance collect - diffusion, and are slowed dow neighboring par	comprehensive theory - simulation - experimental study of collective and self - pensions of charge - stabilized colloidal spheres [1]. In simulation and theory, the et by a hard - core plus screened Coulomb pair potential. Intermediate and self - cattering functions are calculated from accelerated Stokesian Dynamics simulations namic interactions (HIs) are fully accounted for. The study spans the range from the the colloidal long - time regime. Additionally, Brownian Dynamics simulation and g theory (MCT) results are generated where HIs are neglected. It is shown that HIs tive and self - diffusion at intermediate and long times, whereas at short times self for wavenumbers outside the structure factor peak region also collective diffusion wn. MCT significantly overestimate the slowing influence of dynamic caging by rticles.	

The simulated scattering functions are in good agreement with dynamic light scattering (DLS) results for suspensions of charged silica spheres in a refractive index - matched organic solvent mixture. Simulation and theoretical results are indicative of a long - time exponential decay of the intermediate scattering function. The approximate validity of a far - reaching time - wavenumber factorization of the intermediate scattering function observed experimentally [2] is shown to be a consequence of HIs. The study of collective diffusion is amended by simulation and theoretical results for the self - intermediate scattering function and its leading order non - Gaussian parameter, and for the mean squared displacement (MSD) and its time derivative. Since self - diffusion is not assessed in standard DLS measurements, a method to deduce the MSD approximately using DLS is theoretically validated.

References:

 A.J. Banchio, M. Heinen, P. Holmqvist and G. Nägele, Short- and long - time dynamics, and dynamic scaling in suspensions of charged colloidal particles, J. Chem. Phys. 148, 134902 (2018).
 P. Holmqvist and G. Nägele, Phys. Rev. Lett. 104, 058301 (2010).

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Structure Formation due to Antagonistic Salts

Antagonistic salts are composed of hydrophilic and hydrophobic ions. In a mixture solvent (wateroil) such ion pairs are preferentially attracted to water or oil, giving rise to a coupling between the charge density and the composition.

First, they form a large electric double layer at a water-oil interface, reducing the surface tension and producing mesophases. Here, the cations and anions are loosely bound by the Coulomb attraction across the interface on the scale of the Debye screening length. Second, on solid surfaces, hydrophilic (hydrophobic) ions are trapped in a water-rich (oil-rich) adsorption layer, while those of the other species are expelled from the layer. This yields a solvation mechanism of local charge separation near a solid.

We predict a first-order surface phase transition of an electric double layer composed of an antagonistic salt in a mixture solvent on an electrode in electric field.

References:

- [1] A. Onuki, S. Yabunaka, T. Araki, R. Okamoto, Current Opinion in Colloid, Interface Science 22, 59-64 (2016).
- [2] S. Yabunaka and A. Onuki, PRL 119, 118001 (2017).

16:50 - 17:30 **Jure Dobnikar** (Univ. of Cambridge, UK, Chinese Acad. of Sciences, China)

Soft physics of hard materials: non-equilibrium self-assembly in cement hydration

Coauthor(s):

K. Ioannidou [3], M. Kanduc [4], L. Li [2], D. Frenkel [2], E. Del Gado [5]

[2] Department of Chemistry, University of Cambridge [3] Department of Civil and Environmental Engineering, Massachusetts Institute of Technology, Cambridge, USA [4] Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany [5] Department of Physics and Institute for Soft Matter Synthesis and Metrology, Georgetown University, Washington, USA

Perhaps surprisingly, soft matter processes at the nanoscale crucially determine macroscopic mechanic properties and long-term evolution of common materials such as cement. During cement hydration, the dynamic physico-chemical environment dictates the evolution of the structure and effective interactions between nanoscopic building blocks. Here we use Monte Carlo and Molecular Dynamics simulations to study a coarse-grained model of this complex process comprised of colloidal nanoparticles with effective short-range attraction and long-range repulsion [1].

We observe that the structure and symmetry of the growing clusters strongly depends on the time evolution of the effective interactions during the non-equilibrium assembly process and map out the "dynamic phase diagram". The two distinct pathway towards the final dense structure are via i) the formation of finite size isotropic clusters and ii) the growth of elongated clusters and percolated gel-like structures. The unique strength of cement is attained only with a proper balance between the early-stage gel formation and the continuous densification of the material.

Our understanding of non-equilibrium self-assembly enable designing kinetic pathways for material optimization not only in cement but likely also in several other processes such as protein

aggregation or biomineralization. However, for further progress it is urgent to better understand electrostatic interactions in complex time-dependent environments.

References:

 K. Ioannidou, M. Kanduc, L. Li, D. Frenkel, J. Dobnikar, E. Del Gado, Crucial effect of early-stage gelation on mechanical properties of cement, Nature Communications 7 12106 (2016)

Tuesday, September 25, 2018

09:00 - 09:40

Alan Denton (North Dakota State University, USA)

Coarse-grained modeling of macroionic mixtures: Colloids, nanoparticles, and microgels

Interparticle interactions and bulk properties of colloidal suspensions can be substantially modified by addition of nanoparticles. Extreme asymmetries in size and charge between colloidal particles and nanoparticles present severe computational challenges to molecular modeling. I will outline a statistical mechanical theory of effective electrostatic interactions, based on a sequential coarsegraining procedure, which allows a multicomponent mixture of charged colloids, nanoparticles, and microions to be mapped first onto a binary mixture of colloids and nanoparticles [1] and then onto a one-component model of pseudo-colloids [2]. In a linear-response approximation, the onecomponent model is governed by a single effective pair potential and a one-body volume energy, whose parameters depend nontrivially on nanoparticle size, charge, and concentration. To test the theory and to explore the influence of charged nanoparticles on the structure of charge-stabilized colloidal suspensions, we have performed molecular dynamics simulations. For moderate electrostatic couplings, colloid-colloid radial distribution functions and static structure factors agree closely between the one- and two-component models, validating the sequential coarsegraining approach. Analysis of structural properties shows that increasing the charge and concentration of nanoparticles progressively weakens correlations between charged colloids due to enhanced screening of electrostatic interactions, promoting melting of colloidal crystals and aggregation of colloids [3].

lonic microgels are soft colloidal particles composed of cross-linked polymer networks that swell and can acquire charge when dispersed in a solvent. The equilibrium size of a swollen microgel depends on a delicate balance of elastic and electrostatic osmotic pressures, which can be tuned by varying internal particle properties and external environmental conditions, such as temperature, pH, ionic strength, and concentration. The compressibility of these soft particles results in unusual bulk behavior compared with hard-sphere colloidal suspensions. Because of their tunable properties and ability to encapsulate drug or dye molecules, microgels have many practical applications, e.g., for drug delivery, biosensing, filtration, tissue engineering, and carbon capture. Considering the many degrees of freedom of soft macroions, large-scale molecular modeling can be computationally challenging. I will summarize our recent efforts to describe suspensions of ionic microgels within comprehensive coarse-grained models that combine the polymeric and colloidal natures of the particles [4-6]. The models synthesize the internal free energy of polymer gels with effective elastic and electrostatic interactions between permeable, compressible, charged spheres. I will present illustrative results, computed from Monte Carlo and molecular dynamics simulations and from Poisson-Boltzmann and thermodynamic perturbation theories, for equilibrium thermodynamic and structural properties at concentrations ranging from dilute to beyond particle overlap.

- [1] Jun Kyung Chung and Alan R. Denton, "Effective electrostatic interactions in mixtures of charged colloids," Phys. Rev. E 88, 022306 (2013).
- [2] Alan R. Denton, "Effective electrostatic interactions in colloid-nanoparticle mixtures," Phys. Rev. E 96, 062610 (2017).
- [3] Braden M. Weight and Alan R. Denton, "Structure and stability of charged colloid-nanoparticle mixtures," J. Chem. Phys. 148, 114904 (2018).
- [4] Tyler J. Weyer and Alan R. Denton, "Concentration-dependent swelling and structure of ionic microgels: Simulation and theory of a coarse-grained model," Soft Matter (2018).
- [5] Alan R. Denton and Qiyun Tang, "Counterion-induced swelling of ionic microgels," J. Chem. Phys. 145, 164901 (2016).
- [6] Matthew Urich and Alan R. Denton, "Swelling, structure, and phase stability of compressible microgels," Soft Matter 12, 9086 (2016).

09:40 - 10:20 Jan-Philip Machtens (ICS-4, Forschungszentrum Jülich, Germany)

Anion conduction and secondary active glutamate transport at atomic resolution

The lipid bilayer is a perfect electrical insulator and provides the basis for molecular information processing at the cell membrane. Electrical signaling requires both ion-selective and dynamically regulated membrane permeabilities as well as specific concentration gradients across the membrane. Ion channels contain molecular pores that selectively permit certain ions to passively flow across the cell membrane along their electrochemical potential gradients; in contrast, active transporters pump solutes against their gradients.

The core of ion channel and transporter function, the actual transport process across the membrane, is an inherently dynamic process and thus challenging to track with static structural studies only. Molecular dynamics (MD) computer simulations have been successfully used to study mechanisms of ion channels and transporters. By directly simulating ion permeation in channels or partial reactions of transporter function, state-of-the-art molecular simulation techniques can provide quantitative predictions of experimentally accessible properties (e.g. single-channel conductance or selectivity of ion channels). Thereby, the combination of experiment and simulation can provide validated insights into the detailed motions of individual atoms and ions underlying membrane transport with high spatial and temporal resolution, which would have been impossible with experimental approaches alone [1-3].

Excitatory amino acid transporters (EAATs) terminate glutamatergic synaptic transmission and control synaptic glutamate concentrations by moving the transmitter back from the synaptic cleft into surrounding cells. EAATs do not only represent the main glutamate re-uptake system in the mammalian brain; but they are also ligand-gated anion channels [4,5]. Anion channel opening can only occur in certain transporter conformations, resulting in an intimate coupling of glutamate transport and anion channel function. Using a combination of all-atom molecular dynamics simulations and patch-clamp experiments, we identified how EAATs transport glutamate, how they serve as anion-conducting channels, and how these channels open and close, with the ultimate aim to understand how EAAT transport and channel function are coupled to each other [6]. Consequently, we will use our results to identify novel intermediate EAAT structures as potential drug targets and search for conformation-selective pharmacological agents. These studies might

establish a basis for future correction of EAAT glutamate transport and anion conduction under pathological conditions.

References:

- Kutzner, C., Köpfer, D. A., Machtens, J. P., de Groot, B. L., Song, C. & Zachariae, U. Insights into the function of ion channels by computational electrophysiology simulations. Biochim. Biophys. Acta 1858:1741-1752 (2016).
- [2] Vickery, O. N., Machtens, J. P., Tamburrino, G., Seeliger, D. & Zachariae, U. Structural Mechanisms of Voltage Sensing in G Protein-Coupled Receptors. Structure 24:997-1007 (2016).
- [3] Machtens, J. P., Briones R., Alleva C., de Groot B. L., Fahlke Ch. Gating Charge Calculations by Computational Electrophysiology Simulations. Biophysical Journal 112(7):1396-1405 (2017).
- [4] Fahlke, Ch., Kortzak, D. & Machtens, J. P. Molecular physiology of EAAT anion channels. Pflügers Arch 486(3), 491-502 (2016).
- [5] Ewers, D., Becher, T., Machtens, J. P., Weyand, I. & Fahlke, Ch. Induced fit substrate binding to an archeal glutamate transporter homologue. Proceedings of the National Academy of Sciences of the United States of America 110, 12486-12491 (2013).
- [6] Machtens, J. P., Kortzak, D., Lansche, C., Leinenweber, A., Kilian, P., Begemann, B., Zachariae, U., Ewers, D., de Groot, B. L., Briones, R. & Fahlke, Ch. Mechanisms of anion conduction by coupled glutamate transporters. Cell 160, 542-53 (2015).

10:50 - 11:30

Jérome Crassous (Lund University, Sweden / RWTH Aachen, Germany)

Phase behaviour and assembly of bowl-shaped colloids

Charged fluorescent bowl-shaped colloids consisting of a polystyrene core surrounded by a poly(Nisopropylacrylamide) shell were obtained by nanoengineering spherical composite microgels [1]. First, their phase diagram is explored under deionized conditions using confocal microscopy. Hereby, we support the different structural transitions from a fluid to a plastic crystal phase, with freely rotating particles, followed by a glassy state by assessing the influence of the bowl-shape on the structural and dynamical properties of the dispersions. We further demonstrate the use of these responsive bowl-shape colloids to implement an externally controllable lock and key selfassembly mechanism with oppositely charged complementary microgel particles. The dynamic nature of the association allows to reversible cycle through various structures that range from weakly structured dense liquids to well-defined molecule -shaped clusters with different configurations through variations in temperature and ionic strength [2]. We link this complex and dynamic self-assembly behaviour to the relevant molecular interactions such as screened Coulomb and van der Waals forces and the geometrical complementarity of the two building blocks.

References:

- [1] J.J. Crassous et al., Nanoscale, 2015, 7, 15971-15982
- [2] A.M. Mihut et al., Sci. Adv., 2017, 3, e1700321

Christios N. Likos, University of Vienna, Austria)

Electric-field driven self-assembly of ionic mogrogels

Coauthor(s):

11:30 - 12:10

Thiago Colla [1], Priti Mohanti [2,3], Sofi Nöjd [3], Erik Bialik [3], Aaron Riede [3], Peter Schurtenberger [3]

[1] Instituto de Física, Universidade Federal de Ouro Preto, CEP 35400-000 Ouro Preto, Minas Gerais, Brazil; [2] School of Chemical Technology, Kalinga Institute of Industrial Technology (KIIT), Bhubaneswar 751024, India; [3] Division of Physical Chemistry, Lund University, SE-221 00 Lund, Sweden

The structural properties of a system of ionic microgels under the influence of an alternating electric fi eld are investigated both theoretically and experimentally. This combined investigation aims to shed light on the structural transitions that can be induced by changing either the driving frequency or the strength of the applied fi eld, which range from string-like formation along the fi eld to crystal-like structures across the orthogonal plane.

In order to highlight the physical mechanisms responsible for the observed particle self-assembly, we develop a coarse-grained description, in which eff ective interactions among the charged microgels are induced by both equilibrium ionic distributions and their time-averaged hydrodynamic responses to the applied fi eld. These contributions are modeled by the buildup of an eff ective dipole moment at the microgels backbones, which is partially screened by their ionic double layer. We show that this description is able to capture the structural properties of this system, allowing for very good agreement with the experimental results. The model coarse-graining parameters are indirectly obtained via the measured pair distribution functions and then further assigned with a clear physical interpretation, allowing us to highlight the main physical mechanisms accounting for the observed self-assembly behavior.

References:

 Thiago Colla, Priti S. Mohanty, Sofi Nöjd, Erik Bialik, Aaron Riede, Peter Schurtenberger and Christos N. Likos, Self-Assembly of Ionic Microgels Driven by an Alternating Electric Field: Theory, Simulations and Experiments, ACS Nano 12, 4321-4337 (2018). DOI: 10.1021/acsnano.7b08843

13:40 - 14:20	Malin Zackrisson Oskolkova (Novo Nordisk A/S, Denmark)		
Self-associatin	ng proteins		
<u>Coauthor(s):</u> Johan Bergenho [1] Department	<u>Coauthor(s):</u> Johan Bergenholtz [1] [1] Department of Chemistry and Molecular Biology, Gothenburg University, Sweden		
Self-associating interactions [1]. in origin. This g systems. Under associating pro- increasing the p antibacterial po	proteins assemble via strongly anisotropic or patchy attractive protein-protein . The interaction itself is non-covalent and can be electrostatic and/or hydrophobic gives rise to specific protein complexes which are commonly found in biological r specific solution conditions in terms of pH and ionic strength, one such self- tein, lactoferrin (LF), associates into dimers and higher- order oligomers upon protein concentration. We address the structure-function relationship of lactoferrin tency in light of the strong tendency of LF to oligomerize [2], by performing some sed to assess antibacterial effectiveness. As protein diffusion is a central quantity		

in some of these tests, the collective diffusion coefficient has been examined experimentally as a function of concentration [3]. In comparison with particles interacting with isotropic interactions the LF collective diffusion coefficient shows an atypical behavior with two distinct concentration regimes where the collective diffusion coefficient is a decreasing function of LF concentration. The results for the diffusion coefficient along with results for the structure factor from static light and X-ray scattering [4] are interpreted in terms of a theoretical framework for self-associating systems formulated as an integral equation theory by Wertheim in the 1980s [5]. Based on this the first concentration regime seen in the collective diffusion coefficient is suggested to be caused by a monomer-dimer equilibrium whereas the second is interpreted as being caused by further assembly into higher-order oligomers that also serve as precursors for elongated, stripe-like structure formation [6].

References:

- W. Li, B. A. Persson, M. Morin, M. A. Behrens, M. Lund, M. Zackrisson Oskolkova, J. Phys. Chem. B 119, 503 (2015)
- [2] D. Jain, M. Morin, J. Petrlova, M. Zackrisson Oskolkova, J. Bergenholtz, to be submitted.
- [3] W. Li, Attractive patchy protein interactions: understanding of protein dimerization, PhD Dissertation, Lund University, 2016.
- [4] W. Li, B. A. Persson, M. Lund, J. Bergenholtz, M. Zackrisson Oskolkova, J. Phys. Chem. B 120, 8953 (2016)
- [5] M. S. Wertheim, J. Stat. Phys. 35, 35 (1984), J. Chem. Phys. 85, 2929 (1986)
- [6] W. Li, M. Morin, E. Gustafsson, B. A. Persson, M. Lund, M. Zackrisson Oskolkova, Soft Matter 12, 9330 (2016)

14:20 - 15:00 **Roland R. Netz** (Free University of Berlin, Germany)

Testing continuum electrostatic approaches by atomistic simulations

Coauthor(s):

Alexander Schlaich [1], Philip Loche [1] [1] Free University of Berlin

Based on fully atomistic simulations of interacting charged surfaces and ions in water, we discuss the validity of continuum models for the dielectric response at interfaces and for the interaction between charged surfaces. For this, we use novel MD simulation techniques that allow to efficiently perform simulations at constant water chemical potential.

For the electrostatic energy of an ion in the vicinity of a surface we find the electrostatic contribution to be dominated by the non-electrostatic contribution. Linear dielectric theory breaks down, and to quantitatively describe the linear dielectric contribution an anisotropic tensorial dielectric model is needed.

For the interaction between planar charged surfaces we find a modification of the Poisson– Boltzmann equation necessary that includes finite-range ion–surface interaction potentials, while effects due to dielectric profiles and the smeared-out external charge distribution is negligible. For not too high charge, the surface–surface interaction can be explained by the superposition of hydration repulsion and the pressure from Poisson–Boltzmann theory.

15:30 - 16:10 **Alexey Eremin** (University of Magdeburg, Germany)

Structure and dynamics in a fibrillose organoferrogel containing mobile MNPs

Since ferrogels have proved to be magnetoresponsive composite materials they became the focus of intensive research. [1] Low molecular weight gelators such as 12-HOA enable simple preparation of organoferrogels. We use 12-HOA as a gelator known to form an LC phase with helical nanofilaments in mixtures with oils. In the gelator fibres, the dimers are packed in a fashion resulting in twisted layers as reported for bent-core mesogens. [2]

We present structural and magnetooptical studies of gels doped with magnetic nanoparticles (MNPs). These gels are distinguished by a network of twisted nanofibres confining the dynamics of the MNPs. The gels exhibit a strong optical hysteresis of birefringence depending on the magnetic field. It results from the interaction between the magnetic fluid subphase and the fibre scaffold. Those interactions restrict the dynamics of the MNPs. Using various spectroscopy techniques, we analyse the diffusion of the MNPs and magnetic relaxation in the gel matrix. We compare these responses in isotropic and anisotropic gels and discuss the effects of confinement.

References:

[1] M. Zrinyi, L. Barsi, and A. Büki, Polymer Gels and Networks, 5, 415, (1997).

[2] M. Laupheimer, N. Preisig, C. Stubenrauch, J. Chem. Phys. 142, 204905 (2015).

16:10 - 16:50 **Frank Schreiber** (University of Tübingen, Germany)

Tuning Protein Behavior by Multivalent Charges: Aggregation, Diffusion, and Adsorption

We discuss concepts for controlling and understanding protein aggregation pathways and the branching between them in aqueous solution by addition of multivalent ions. This route for the tailoring of the interaction potential is exploited for controlling a) crystallization, b) gelation and amorphous aggregation, as well as c) smaller aggregate formation including their dynamics and kinetics. Furthermore, we discuss the connection to and the role of interfaces in this context.

First, we present a real-time study of protein crystallization induced by multivalent ions using small-angle scattering and optical microscopy. Based on the crystallization kinetics, we propose a multistep mechanism. In the first step, an intermediate phase is formed, followed by the nucleation of crystals within the intermediate phase. During this period, the number of crystals increases with time, but the crystal growth is slowed down by the surrounding dense intermediate phase due to the low mobility.

In the next step, the intermediate phase is consumed by nucleation and slow growth, and the crystals are exposed to the dilute phase. In this stage, the number of crystals becomes nearly constant, whereas the crystals grow rapidly due to access to the free protein molecules in the dilute phase. This real-time study not only provides evidence for a two-step nucleation process for protein crystallization, but also sheds light on the role and the structural signature of the metastable intermediate phase in this process.

Furthermore, the competing routes of aggregation are elucidated, as is the role of the general features of the phase diagram including liquid-liquid phase separation (LLPS).

Second, we present complementary investigations of the dynamics of these systems using quasielastic neutron scattering, showing a remarkably universal behaviour of the effective diffusion as a function of concentration and salt under suitable conditions.

Third, we show how these concepts can be transferred to protein-interface interations, and how adsorption behavior can be manipulated by multivalent charges. We try to connect the interface and the bulk behavior, including reentrant adsorption and anomalous interface behavior upon approaching bulk phase boundaries.

Finally, we comment on the role of specific ions and attempt a comprehensive discussion of models and theories suitable for a comprehensive explanation of these phenomena.

References:

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- [4] F. Roosen-Runge et al., Nature Scientific Reports (2014)
- [5] F. Roosen-Runge et al., PNAS (2011)
- [6] M. R. Fries et al., Phys. Rev. Lett. (2017)

16:50 - 17:30

Peter Fischer (ETHZ, Zurich, Switherland)

The salt curve revisited: Electrostatic charges govern the viscoelastic properties of micellar solutions

In ionic surfactant micelles, interactions among surfactant monomers, their counterion, and additives are fundamental to tune molecular self-assembly and thus the rheological properties (see Figure 1). Here we propose a combination of 1H-NMR, integrated small-angle neutron scattering (SANS) and small-angle X-ray scattering, and rheology to probe the molecular arrangements of the individual molecules within the micelle and the resulting flow properties [1-3]. Shifts in the 1H-NMR signal show the penetration of counterions and additives into the micellar surfactant structure while SANS and SAXS determine specific intramicellar length scales and intermicellar interactions. SANS signals are sensitive to the contrast between the solvent (deuterium) and the hydrocarbonic tails in the micellar core (hydrogen) and SAXS access the inner structure of the polar shell because the headgroups, counterions, and penetrated salt have higher electron densities compared to the solvent and to the micellar core. The number density, intermicellar distances, aggregation number, and inter/intramicellar repulsions are discussed on the basis of the dependence of the structure factor and form factor on the micellar aggregate morphology. The results allow us to propose a modified packing parameter model taking electrostatic charges into account. As a consequence, micellar growth and structure can be discussed by variations in the flexibility and size of the headgroup as well as the ionic dissociation rate of its counterion. Additionally, we show that the counterion binding is even more significant to the development of viscoelasticity than the headgroup structure of a surfactant molecule [2, 4, 5]. This somewhat surprising finding shows the importance of electrostatic charges in the self-assembly process and its consequences on the rheological fingerprint of viscoelastic surfactant solutions.

References:

- [1] V. Lutz-Bueno, R. Pasquino, M. Liebi, J. Kohlbrecher, P. Fischer: Langmuir 32 (2016) 4239
- [2] V. Lutz-Bueno, M. Liebi, J. Kohlbrecher, P. Fischer: Langmuir 33 (2017) 2617
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- [4] V. Lutz-Bueno, J. Zhao, R. Mezzenga, T. Pfohl, P. Fischer, M. Liebi: Lab Chip 16 (2016) 4028
- [5] V. Lutz-Bueno, R. Pasquino, S, Haward, A. Shen, P. Fischer: J. Rheol. 61 (2017) 769

Wednesday, September 26, 2018

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Orlin D. Velev (North Carolina State University, USA)

Ionic motility in active soft matter: Particle systems that translate, rotate, and interact through electrokinetic effects

The focus of this talk will be the principles of using ionic mobility to achieve active particle propulsion. The properties of the ionic counterlayers are determining the stability of numerous colloidal and soft matter systems [1]. Electrokinetic effects of ionic charge transport in particle and soft matter systems can be used in hydrogel circuits [2,3] and soft robotics [4,5]. Here, we will specifically discuss how directional ionic mobility initiated and directed by AC electric fields can endow different classes of particles with the ability to operate as "active" colloidal systems. Typically, this requires the breaking of the particle symmetry and polarization pattern, such as making metallo-dielectric particles by design [6,7]. The rich variety of mechanisms of motility in such active systems include electrohydrodynamic flows, reversed electrohydrodynamic flows, induced charge electrophoresis, and self-dielectrophoresis [8]. These mechanisms will be exemplified with a new class of microspinners that display three frequency-triggered directional spin inversions. Lastly, we will introduce a class of active semiconductor microparticles that draw energy from external AC electric fields to self-propel in a controlled direction [9,10]. Such motile silicon particles can be comprehensively designed with microfabrication tools and can have future applications such as microsensors, artificial muscles, reconfigurable neural networks and computational systems. We will discuss how a combination of electrokinetic effects, such as surface electroosmosis, induced charge electrophoresis, and dielectrophoresis, can controllably drive the semiconductor microparticle motion, interactions and collective dynamics [11].

References:

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	Jens Harting (Helm
09:40 - 10:20	Forschungszentrum

holtz Institute Erlangen-Nürnberg, n Jülich, Germany)

Mesoscopic electrohydrodynamic simulations of multiphase flows

We recently developed a computational model to simulate electrokinetic phenomena involving multiphase fluid flows and colloidal suspensions. The method is based on a pseudopotential lattice Boltzmann method for multiphase flows. The Nernst-Planck equation, describing the kinetics of dissolved ion species, is solved using a finite volume discretization based on the link-flux method. Suspended colloids are resolved on the lattice and coupled to the hydrodynamics and electrokinetics through appropriate boundary conditions [1].

We will present the integration of the method and some validation cases.

Its possibilities are explored by considering various physical systems, such as breakup of charged and neutral droplets and colloidal dynamics at either planar or spherical fluid interfaces. Then, we focus on electrowetting of nanodrops of aqueous electrolyte mixtures. We report a new method for controlling the degree of deformation and minimum attainable contact angle by varying the difference of solvation strengths between the two solvents, which determines the ratio of ion concentrations [2].

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10:50 - 11:30

Emmanuel Trizac (Université Paris-Sud, France)

Advances in the strong coupling theory for counter-ions distributions

Coauthor(s):

M. Trulsson [1], L. Samaj [2]

[1] Lund University, [2]Slovak Academy of Sciences

We study thermal equilibrium of counterions confined between symmetrically charged walls at distance d. Existing analytical approaches are either restricted to the mean-field limit (weak-coupling), or to the strong-coupling regime provided that d is not too large.

At very large couplings when the counterion system is in its crystal phase, a harmonic expansion of particle deviations is made around the bilayer positions, with a free lattice parameter determined from a variational approach. For each of the two walls, the harmonic expansion implies an effective one-body potential at the root of all observables of interest in our Wigner strongcoupling expansion. Analytical results for the particle density profile and the pressure are in remarkable agreement with numerical Monte Carlo data, for small as well as intermediate values of d comparable with the Wigner lattice spacing. While the strong-coupling theory is extended to the fluid regime by using the concept of a correlation hole, the Wigner calculations appear trustworthy for all electrostatic couplings investigated.

Our results significantly extend the range of accuracy of analytical equations of state for strongly interacting charged planar interfaces.

References: [1] Soft Matter 14, 4040 (2018)

11:30 - 12:10

Ben Werkhoven (Utrecht University, The Netherlands)

Electrokinetic problem of a pressure-induced liquid flow through a narrow long channel

Coauthor(s):

Rene Van Roij [1],

[1] Utrecht University, The Netherlands

We theoretically study the electrokinetic problem of a pressure-induced liquid flow through a narrow long channel with charged walls, going beyond the classical Helmholtz-Schmolukowski picture by considering the surprisingly strong combined effect of (i) Stern layer conductance and (ii) dynamic charge-regulating rather than fixed surface charges. We find that the water flow induces, apart from the well-known streaming potential, also a strongly heterogeneous surface charge and zeta-potential on chemically homogeneous channel walls. Moreover, we identify a novel steady state with a nontrivial 3D electric flux with 2D surface charges acting as sources and sinks. For a pulsed pressure drop our findings also provide a first-principles explanation for ill-understood experiments on the effect of flow on interfacial chemistry [D. Lis et al., Science 344, 1138 (2014)]. If time permits, we will discuss some recent work where we reproduce the equilibrium contact angle of a water droplet in a decane-stearic acid solution, which was shown to be very ion specific and salinity dependent.

13:40 - 14:20

Filip Strubbe (Ghent University, Belgium)

Charging phenomena at interfaces with surfactant-doped nonpolar liquids

The electrical charge of surfaces in contact with surfactant-doped nonpolar liquids plays an important role in applications such as electronic ink displays and liquid toner printing. On the one hand pigment particles dispersed in a nonpolar liquid containing surfactant become charged as a result of interactions with surfactant aggregates (inverse micelles). And on the other hand the electrode interfaces, which are often coated by dielectric layers, can become charged through interactions with charged inverse micelles.

Here, several studies are reported aiming to elucidate the way inverse micelles interact with and electrically charge solid-liquid interfaces in nonpolar liquids. Firstly, Millikan-type of measurements of the electrical charge of individual particles in surfactant-doped nonpolar liquids are carried out with precision higher than the elementary charge [1,2]. Depending on the surfactant concentration, phenomena such as field-induced charging or charge regulation are observed. Secondly, the retardation effect during electrophoresis of single particles is investigated for the case that the diffuse double layer consists of charged inverse micelles [3]. By optical trapping of individual particles and by applying an electric field, the double layer is effectively stripped-off, thereby reaching the Hückel limit. The mobility measured for intermediate stripping of the doublelayer is analyzed using simulations of the local micelle concentrations. Thirdly, it is shown that, depending on their size, inverse micelles interact differently with solid interfaces [4,5]. Usually, large inverse micelles bounce off interfaces and form a diffuse double layer in the presence of a field, whereas small micelles tend to adsorb to interfaces forming a thin Stern layer. However, an interesting exception is demonstrated for the case of large charged inverse micelles generated in the presence of an electric field which also appear to adsorb to the interface [6]. And finally, with experiments and simulations it is investigated how charge at the interfaces influences the dynamics of the electric field and particle concentrations when various voltage signals are applied [7-9].

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14:20 - 15:00 Vania Calandrini (IAS-5/INM-9, Forschungszentrum Jülich, Germany)

From atomistic simulations to collective transport phenomena at neuronal membranes: preliminary results by a Generalized Langevin Equation approach

Neurotransmission is driven by molecular signaling cascades, mediating very complex processes, such as memory, learning, mood etc. Knowing how key physicochemical features, such as geometrical constraints, membrane composition, diffusion processes, mutations, crowding or electric fields, combine together and shape over time and space neuronal signaling would provide important hints on the human brain functioning.

Here we present preliminary results about a mesoscale modeling of post-synaptic signalling events based on Generalized Langevin dynamics, which aims at dissecting the interplay among all these aspects. This approach provides the ideal framework to model transport phenomena occurring at the neuronal membrane, which cannot be modeled within currently available approaches based on standard Brownian Dynamics.

The generalized friction of a macromolecule in a specific lipid bilayer at infinite dilution is derived in a mean field-like approach by higher resolution simulations. In the current

implementation, explicit inter-macromolecular interactions (such as electrostatic interactions), which may be relevant at finite macromolecular concentrations, are not included yet.

15:30 - 16:10 **Paolo Carloni** (INM-9 & IAS-5, Forschungszentrum Jülich, Germany)

Ligands binding to nucleic acids: insights from molecular simulation

We will present results from recent molecular simulation studies on DNA's and RNA's binding to proteins and small molecules. The relevance of electrostatic interactions in the binding process will be highlighted. The limitations of the methods used (molecular dynamics simulations and free energy calculations) will be discussed.

References:

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Emanuela Bianchi (University of Vienna / TU Wien, Austria)

Tuning the order of colloidal monolayers: assembly of heterogeneously charged colloids close to a substrate

We study the behavior of negatively charged colloids with two positively charged polar caps close to a planar patterned surface. We consider substrates composed of alternating (negative/neutral, positive/neutral and positive/negative) parallel stripes and, by means of Monte Carlo simulations, we investigate the ordering of the colloids on changing the number of the stripes. The competition between the different anisotropic components of the particle-particle interaction patterns is able by itself to give rise to a rich assembly scenario: colloids with charged surface patterns form different crystalline domains when adsorbed to a homogeneously charged substrate. Here we show that the additional competition between the two different lengths scales characterizing the system (i.e., the particle interaction range and the size of the stripes) gives rise to a plethora of distinct particle arrangements, where some well-defined trends can be observed. By accurately tuning the substrate charged motif it is possible to favor the formation of, e.g., specific crystalline domains, elongated compact clusters or extended particle networks.

16:50 - 17:30

Clemens Jochum (TU Wien, Austria)

Structure and stimuli-responsiveness of all-DNA dendrimers: theory and experiment

Coauthor(s):

Nataša Adžić[1], Emmanuel Stiakakis[2], Gerhard Kahl[3], Christos N. Likos[1] [1] University of Vienna, Austria [2] Forschungszentrum Jülich, Germany [3] TU Wien, Austria

We present a comprehensive theoretical and experimental study of the solution phase properties of DNA-based family of nanoparticles - dendrimer-like DNA molecules (DL-DNA) [1]. These charged DNA dendrimers are novel macromolecular aggregates, which hold high promise in targeted selfassembly of soft matter systems in the bulk and at interfaces. To describe the behavior of this family of dendrimers, we use a theoretical model in which base-pairs of a single DL-DNA molecule are modeled by charged monomers, whose interactions are chosen to mimic the equilibrium properties of DNA correctly. Experimental results on the sizes and conformations of DL-DNA are based on static and dynamic light scattering; at the same time, Molecular Dynamics simulations are employed to model the equilibrium properties of DL-DNA, which compare favorably with the findings from experiments while at the same time providing a host of additional information and insight into

the molecular structure of the nanostructures. We also examine the salt-responsiveness of these macromolecules. The study of these charged dendrimer systems is an important field of research in the area of soft matter due to their potential role for various interdisciplinary applications, ranging from molecular cages and carriers for drug delivery in a living organism [2] to the development of dendrimer- and dendron-based ultra-thin films in the area of nanotechnology [3].

These findings are essential to determine if DL-DNA is a viable candidate for the experimental realization of cluster crystals in the bulk, a novel form of solids with multiple site occupancy [4].

References:

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Thursday, September 27, 2018

09:00 - 09:40

Daniel Hammer (University of Pennsylvania, USA)

The dynamics and stability of droplets made from recombinant coacervating charged proteins

Materials made from recombinant proteins offer precision in molecular weight and sequence, which is the key to biofunctionality. We have been making families of recombinant proteins that have the ability to phase separate into protein rich liquid droplets. One of these is based on the intrinsically disordered protein LAF-1, which phase separates above a certain concentration. We isolated the active subdomain of the protein – called RGG – and dimerized it. We found that the dimer phase separates, at lower concentrations than the monomer, but that the protein remains mobile in the protein rich phase. By insertion of a protease cleavable domain between the two RGGs, we could reverse phase separation upon addition of a protease, at a rate in which the droplet diameter changes linearly with time. Using zipper domains, we can also attach active proteins to the surface of the drops.

The second is based on the recombinant amphipathic protein oleosin, which has two charged hydrophilic arms and a central hydrophobic core with a proline knot that forces a turn. Thus, the protein is shaped like a "U." We have engineered a subvariant of the oleosin that has 30 amino acids in the central hydrophobic core and has no secondary structure. This surfactant protein migrates to interfaces and can stabilize

emulsion droplets and bubbles. At low concentrations, -30- oleosins form spherical micelles, but at high concentrations, they also form liquid droplets. Oleosin has no cysteines; insertion of a cysteine within the N-terminal arms leads to more avid phase separation. Phase separation is permitted at higher temperatures and lower concentrations when cysteines are inserted, with the potency greater as the cysteine is

placed closer to the N-terminus. The additional phase separation is due to disulfide bonding, which can be reversed with a reducing agent.

Both systems allow the construction of interfaces with biological activity, which can easily be achieved using recombinant methods. This activity includes addition of enzymes and protease cleavable domains, light activated assembly, and charged residues.

09:40 - 10:20

Christoph Goegelein (LANXESS GmbH, Germany)

Carbon black reinforced rubber blends with superior crack growth resistance and fatigue lifetime

We study the fatigue properties of cross-linked blends of ethylene propylene diene rubber (EPDM) with low amounts of natural rubber and reinforced with carbon black (CB). These compounds show both high temperature and superior crack growth resistance and fatigue lifetime. For low NR contents, transmission electron microscopy reveals that the NR phase forms small droplets of $20\hat{a}\in$ "50 nm. Remarkably, these droplets are even smaller than the primary CB particles. Atomic force microscopy shows that the NR phase droplets have a higher loss factor and a smaller elastic modulus than the surrounding EPDM matrix. Rheometer measurements are used to study the effect of the phase morphology on the rubber mechanical properties. These rheological data are compared with the prediction of the Eshelby model describing the effect of elastic inclusions on solids. A complex interplay between the rubber phase morphology and the solubility of both the sulfur cross-linking system and CB is observed, which cannot be predicted theoretically. It is proposed that the soft NR droplets effectively inhibit the crack propagation in the EPDM matrix.

10:50 - 11:30 Anselm Horn (Friedrich-Alexander-Univ. Erlangen-Nürnberg, Germany)

Interaction Of Alkali Ions With Fibrillar Amyloid-beta Oligomers

One of the hallmarks in Alzheimer's Disease (AD) is the aggregation of the small amyloid- β (A β) peptide into oligomers and fibrils. Although the notion about the neurotoxic importance of different A β species shifted from unsoluble fibrils to soluble oligomers, which are now believed to be the most neurotoxic species in AD, A β fibrils may serve as a reservoir for small toxic oligomers. It is well known from experiment, that aggregation in general and of A β in particular is modulated by salt in solution e.g. via different concentrations or the nature of the ions. The molecular details of the underlying interactions, however, are still not fully understood.

In physiological environments, salts occur ubiquitously and are known to have profound effects on the solubility of proteins (Hofmeister series). Monovalent alkali metal ions, however, seem to exhibit a more subtle effect on A β aggregation in experiment than higher charged species [1, 2]. Here, we investigate the interaction of different alkali metal ions with fibrillar A β oligomers of different size by means of molecular dynamics (MD) simulations. For a systematic series of single and double layer fibrillar A β oligomers MD simulations were conducted within an aqueous environment containing LiCl, NaCl, and KCl. Thus, we study the presence of the so-called 'sodiumeffect' in amyloid structures. Originally, this effect was described for dendrimer micelles formation modulating the self-organization of amphiphilic carboxylates: Na+ forms bridging complexes with carboxylate groups, in contrast to K+ [3].

Our MD simulations provide insights about the stabilizing interactions between the metal ions and acidic A β key residues (e.g. Glu22). Interestingly, the metal ions enter the A β water channel region via paths suggested in a previous study [4].

References:

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Participants

Austria	 Emanuela Bianchi (University of Vienna / TU Wien) (emanuela.bianchi@univie.ac.at) Clemens Jochum (TU Wien) (clemens.jochum@tuwien.ac.at) Gerhard Kahl (TU Wien) (gerhard.kahl@tuwien.ac.at) Christos N. Likos (University of Vienna) (christos.likos@univie.ac.at)
Belgium	• Filip Strubbe (Ghent University) (<i>filip.strubbe@ugent.be</i>)
Denmark	Malin Zackrisson Oskolkova (Novo Nordisk A/S) (qmzo@novonordisk.com)
France	Emmanuel Trizac (Université Paris-Sud) (trizac@lptms.u-psud.fr)
Germany	 Vania Calandrini (Forschungszentrum Jülich) (v.calandrini@fz-juelich.de) Paolo Carloni (Forschungszentrum Jülich) (p.carloni@fz-juelich.de) Jan Dhont (Forschungszentrum Jülich) (j.k.g.dhont@fz-juelich.de) Alexey Eremin (University of Magdeburg) (alexey.eremin@ovgu.de) Christoph Goegelein (LANXESS GmbH) (christoph.goegelein@lanxess.com) Jens Harting (Helmholtz Institut Erlangen-Nürnberg, Forschungszentrum Jülich) (j.harting@fz-juelich.de) Anselm Horn (Friedrich-Alexander University Erlangen-Nürnberg (anselm.horn@fzu.de) Kyongok Kang (Forschungszentrum Jülich) (k.kang@fz-juelich.de) Wenping Lyu (RWTH Aachen) (wenping.lyu@rwth-aachen.de) Jan-Philip Machtens (Forschungszentrum Jülich) (j.machtens@fz-juelich.de) Gerhard Nägele (Forschungszentrum Jülich) (g.naegele@fz-juelich.de) Roland R. Netz (Free University of Berlin) (rnetz@physik.fu-berlin.de) Frank Schreiber (University of Tübingen)
	Grunk.schreiber wunn-tuebingen.ue)

 Akira Onuki (Kyoto University) (onuki@scphys.kyoto-u.ac.jp) 	
• Ben Werkhoven (Utrecht University) (b.l.werkhoven@uu.nl)	
• Jérome Crassous (Lund University, RWTH Aachen) (jerome.crassous@fkem1.lu.se)	
• Peter Fischer (ETHZ, Zurich) (peter.fischer@hest.ethz.ch)	
• Jure Dobnikar (University of Cambridge, UK, Chinese Academy of Sciences, China) (jd489@cam.ac.uk)	
 Alan Denton (North Dakota State University) (alan.denton@ndsu.edu) Daniel Hammer (University of Pennsylvania) (hammer@seas.upenn.edu) Orlin D. Velev (North Carolina State University) (odvelev@ncsu.edu) 	

Location

The workshop takes place at the TU Wien, "Campus Gusshaus", **1040 Vienna, Gußhausstraße 27-29**



The Venue

Lecture Hall EI 10, ground floor ("Fritz-Paschke-Hörsaal")



Possibilities for Lunch



Austrian Cuisine

(2) Wiener Wiazhaus 1040, Gußhausstraße 24 www.wiener-wiazhaus.at/

(9) Gasthaus am Rilkeplatz 1040, Rilkeplatz 7 01 / 586 61 77

(12) Restaurant Wiener Wirtschaft 1040, Wiedner Hauptstraße 27 01/22 111 364

(x) Cafe-Restaurant
 Resselpark
 1040, Wiedner Hauptstraße 1
 www.restaurant-resselpark.at

Panini & Bagels

(6) Blueorange 1040, Margaretenstraße 9 www.blueorange.co.at

Fusion Cuisine

(1) Salon Wichtig 1040, Karlsgasse 22 http://www.salonwichtig.at/

(7) Point of Sale 1040, Schleifmühlgasse 12-14 www.thepointofsale.at

(11) Fein Essen 1040, Wiedner Hauptstr. 19 www.feinessen.at

Mexican Cuisine

(4) Santos 1040, Favoritenstraße 4-6 www.santos-bar.com

Pizza & Pasta

(3) Riva Pizza Favorita 1040, Favoritenstraße 4-6 www.riva.pizza

(8) Teigware 1040, Rilkeplatz 7/2 www.teigware.at

(10) Mezzo Roma 1040, Rilkeplatz 3 www.mezzo-roma.com

Asian Cuisine

(5) Nagoya Sushi 1040, Schleifmühlgasse 8 www.nagoyasushi-wien.at/

(13) Chang 1040, Waaggasse 1 www.chang.at

Workshop Dinner @ Heuriger "10er Marie"

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How to get there

⇒ With the tram

- Take <u>tram 2</u> from "Karlsplatz/Oper", direction "Dornbach", go to station "Johann-Nepomuk-Berger-Platz"
- Change to tram 44, direction "Ottakring", go to station "Johannes-Krawarik-Gasse"
- The Heurigen is right infront of the station
- ⇒ <u>With the underground</u>
 - Take <u>underground U1</u> from Karlsplatz, direction "Leopoldau", go to station "Stephansplatz"
 - Change to underground U3, direction "Ottakring", go to station "Ottakring"
 - The Heurigen is to reach in a 5 minutes walk, see map below











