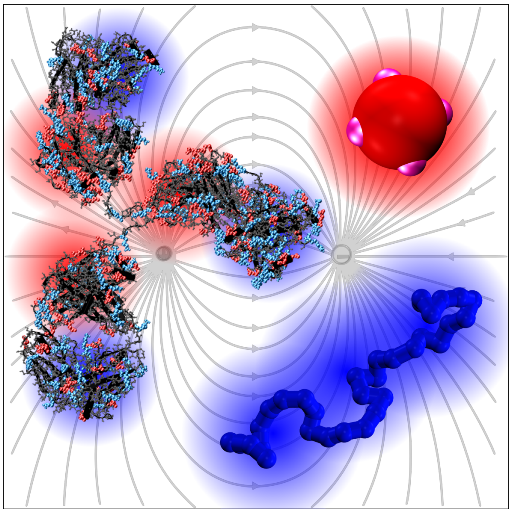
Erwin Schrödinger International Institute
for Mathematics and Physics

Charged Soft Matter:
Bridging Theory and Experiment



Erwin Schrödinger Institute
Vienna, Austria

September 8, 2025 – September 12, 2025

Contents

General Information

Organizing Committee:

Roman Staňo	`rs2365@cam.ac.uk`	University of Cambridge (United Kingdom)
Emanuela Bianchi	`emanuela.bianchi@tuwien.ac.at`	Vienna University of Technology (Austria)
Peter Košovan	`peter.kosovan@natur.cuni.cz`	Charles University (Czechia)
Christos N. Likos	`christos.likos@univie.ac.at`	University of Vienna (Austria)

Venue:

Erwin Schrödinger International Institute for Mathematics and Physics
Boltzmanngasse 9
1090 Wien, Austria

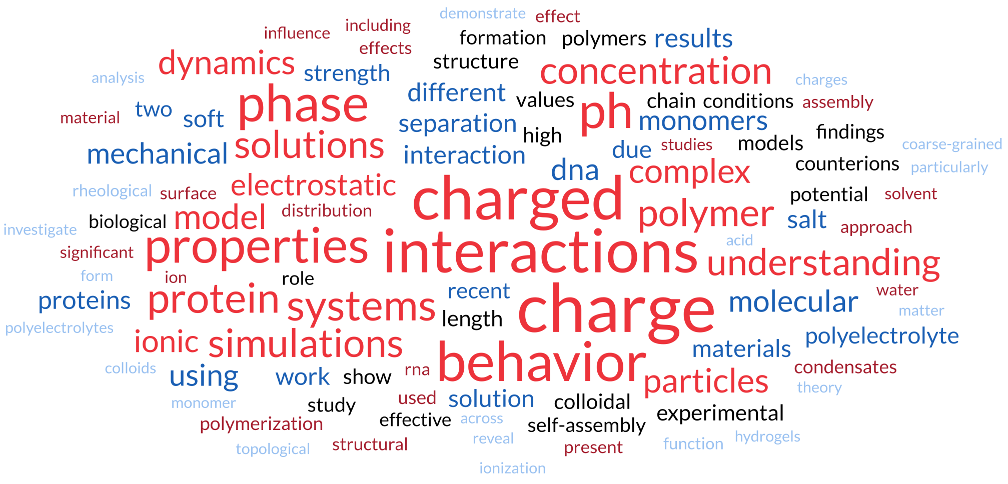
Resources:

workshop website & schedule
https://www.esi.ac.at/events/e571/

lecture recordings
http://www.youtube.com/@ESIVienna

ESI Bluesky account
https://bsky.app/profile/esivienna.bsky.social

ESI Instagram account
https://www.instagram.com/esivienna/



Word cloud showing 100 most frequent words across all of the submitted abstracts, summing up to ∼ 11000 words in total. The font size is proportional to the occurrence. Stop words, numerals and special symbols were removed.

Motivation

Charged Soft Matter entails a broad variety of systems, sharing one common feature: they contain charged macromolecules or colloidal particles, typically few nanometers in size, accompanied by salt ions and other charged small molecules, and polar solvents. The relevant systems range from cellular membraneless organelles to protein solutions, bio-inspired or synthetic polymers, inverse patchy colloids or polymer-electrolytes found in modern battery systems. Although very different in nature, these systems share the same physics, predominantly controlled by interplay of electrostatic interactions and thermal fluctuations.

Unfortunately, most of the research in the field of charged soft matter is carried out in communities centered mainly around the target systems named above, allowing only limited exchange across these communities. This leads not only to differences in nomenclatures and concepts, but also to reinventions and rediscoveries of phenomena. The aim of this workshop is to provide an interdisciplinary platform for scientific exchange between these different communities investigating charged soft matter, underlining the shared aspects of the involved physics.

Class C1: charged colloids, proteins and viruses

This class encompasses synthetic colloidal particles with charged cores [14], Janus particles [15] or heterogeneously charged patchy colloids [2], all of which can exhibit rich phase behavior, clustering or self-assembly. The possession of charges, their distribution on the colloids, but also salt conditions in the colloidal suspensions pose a versatile playground for tuning the effective interactions between the colloids [17], which in turn regulate their collective behavior. Recently, it has been proposed that charged colloids can be also used as a model for globular charged proteins [30], selected viruses [20] or monoclonal antibodies in suspensions [10], as all of these biological objects contain charged regions in geometries akin to synthetic colloids.

Class C2: polyelectrolytes and polypeptides

This class of materials includes polymers, both synthetic and biopolymers, such as DNA or polypeptides, carrying charged functional groups [19, 7]. While colloids and globular proteins are typically rigid objects, polyelectrolytes are flexible molecules, which can attain many different conformations. In contrast to colloids, intramolecular entropy and intramolecular interactions play a major role in polyelectrolyte systems, bringing about unique phase transitions and different modes of dynamics as compared to the colloids. The interplay of flexibility and charge can be even used as a design motif in DNA nanotechnology [24] or as a means to regulate the structure of DNA in concentrated solutions akin to viral genome [28].

Class C3: intrinsically disordered proteins

Intrinsically disordered proteins have entered the spotlight of biochemical research only in recent years. In the past, they have been neglected because they did not fit the established paradigm of lock and key mechanism, relating the protein structure and function. Similar to globular proteins, the disordered ones are built from unique amino acid sequences. Yet, their conformational flexibility makes them similar to polyelectrolytes and synthetic polymers. Therefore, classical polymer theories can describe the structure of individual disordered proteins [13] whereas complexation of highly charged disordered proteins can be described using the same arguments as complexation of polyelectrolytes [6]. Although interactions in disordered proteins are more diverse than in colloids or synthetic polymers, disordered proteins can be considered as a bridge between the previous two classes.

Topic T1: liquid-liquid phase separation and coacervation

Mixing of oppositely charged polyelectrolytes results in phase separation, driven by the entropy of the released counterions, yielding either solid polyelectrolyte complex, or a liquid coacervate [32]. This phenomenon has been systematically investigated using synthetic peptides with custom sequences of acidic (anionic), basic (cationic) and neutral side chains [5, 12], later described using theories previously developed for synthetic polymers [25]. Phase separation is one of the key factors determining the spontaneous compartmentalization in biological systems, leading to the formation of membraneless organelles [9] and enabling selective encapsulation of proteins or other charged solutes not only in biology, but also in artificial bio-inspired systems [4]. The main goal of within this topic is to stimulate the discussion of how the systematic understanding of phase separation and coacervation could be achieved in systems of increasing complexity, up to the level of biological condensates.

Topic T2: self-assembly, structure formation, supramolecular phenomena

Utilizing interactions between charged moieties to form supramolecular structures is a commonly used motif in self-assembly. Oppositely charged blocks of copolymer polyelectrolytes attract each other, forming complex coacervate core micelles [33] in dilute conditions and diverse mesoscopic structures from networks to lamellae or cylindrical phases in concentrated solutions [27]. On the other hand, charge-driven colloidal assembly can lead to formation of ionic solids [14] or cluster crystal phases [29]. While the qualitative ideas behind the above mechanisms are known, the control over this behavior is not quantitative. The main goals within this topic are to discuss how to design supramolecular assemblies from charged soft matter, how to tune the emergent structures, and how to control the processes using external fields or other stimuli.

Topic T3: dynamics, rheology, charge transport and non-equilibrium phenomena

The theoretical understanding of the dynamics of polyelectrolytes and charged colloids in solutions is still an open problem, complicated by the presence of several length scales of hydrodynamic, electrostatic and topological screening [16]. In concentrated phases, polyelectrolytes typically exhibit only weak entanglements and their dynamics is rather fast [8] in spite of crowding, while colloids can exhibit slowdown and features of glassy dynamics. Our main goal within this topic is to shed light on the fundamental principles of dynamics of charged soft matter, and establish parallels between charge transport in natural systems of intrinsically disordered proteins [8], in ionomeric melts [11] and polyelectrolytes in redox-flow batteries [1].

Topic T4: structure and function of soft matter in nature and technology

The central paradigm in molecular biology assumes that the amino acid sequence in proteins determines their structure (spatial organization), and thereby their biological function. This paradigm has been challenged by recent research on disordered proteins and biological condensates (see also Topic T1). On the contrary, colloid and polymer science have traditionally worked with simple particles or chains, composed of repeating identical functional groups, achieving the desired function by tuning the connectivity and shape. Complexity has been introduced in the sequel by using multi-block copolymers, functional side-chains or patchy colloidal particles. Only very recently, colloid theories have been extended to account for structural features [10, 23], bridging the concepts of molecular biology with those of colloid and polymer science. Simultaneously, the function of disordered proteins has been addressed using the concepts from colloid and polymer science [6, 13, 12, 3]. The goal within this topic is to foster this emerging field of research by providing a discussion platform for researchers attempting to bridge these conceptually different approaches to structure and function.

Topic T5: interactions, charge regulation, responsive and programmable matter

The amount of charge on proteins, colloids or polyelectrolytes can be changed by the value of pH in the solution. It is further modulated by a response to changes in the local environment, termed charge regulation. In simple colloids and proteins, charge regulation has been described using the mean-field formalism, based on the Poisson-Boltzmann equation [22, 18]. The same principles apply to charge regulation in polyelectrolytes and short peptides, albeit their conformational flexibility makes the interactions more complex. In a suitably designed system, charge regulation can trigger interactions under specific conditions [21], at a desired location or in time [26]. In the context of biomaterials, a similar effect is termed nanobuffering: a simultaneous change of a charge and conformation of a macromolecule to counterbalance changes in its local environment [31]. The last example underscores the fact that different terminology is used to describe the same physics, depending on the community. Nonetheless, controlling the interactions is the key to controlling the structure, function, phase stability and also dynamical properties. The goal within this topic is to establish a strong connection between the control of electrostatic interactions and the phenomena covered in the previous topics.

[1] L. Bello and C. E. Sing. Mechanisms of diffusive charge transport in redox-active polymer solutions. *Macromolecules*, 53(18):7658–7671, Sept. 2020.

[2] E. Bianchi, R. Blaak, and C. N. Likos. Patchy colloids: state of the art and perspectives. *Physical Chemistry Chemical Physics*, 13(14):6397, 2011.

[3] L. S. Bigman, J. Iwahara, and Y. Levy. Negatively charged disordered regions are prevalent and functionally important across proteomes. *Journal of Molecular Biology*, 434(14):167660, July 2022.

[4] W. C. Blocher McTigue and S. L. Perry. Protein encapsulation using complex coacervates: What nature has to teach us. *Small*, 16(27), May 2020.

[5] L.-W. Chang, T. K. Lytle, M. Radhakrishna, J. J. Madinya, J. Vélez, C. E. Sing, and S. L. Perry. Sequence and entropy-based control of complex coacervates. *Nature Communications*, 8(1), Nov. 2017.

[6] A. Chowdhury, A. Borgia, S. Ghosh, A. Sottini, S. Mitra, R. S. Eapen, M. B. Borgia, T. Yang, N. Galvanetto, M. T. Ivanović, P. Łukijańczuk, R. Zhu, D. Nettels, A. Kundagrami, and B. Schuler. Driving forces of the complex formation between highly charged disordered proteins. *Proceedings of the National Academy of Sciences*, 120(41), Oct. 2023.

[7] A. Dobrynin and M. Rubinstein. Theory of polyelectrolytes in solutions and at surfaces. *Progress in Polymer Science*, 30(11):1049–1118, Nov. 2005.

[8] N. Galvanetto, M. T. Ivanović, A. Chowdhury, A. Sottini, M. F. Nüesch, D. Nettels, R. B. Best, and B. Schuler. Extreme dynamics in a biomolecular condensate. *Nature*, 619(7971):876–883, July 2023.

[9] E. Gomes and J. Shorter. The molecular language of membraneless organelles. *Journal of Biological Chemistry*, 294(18):7115–7127, May 2019.

[10] A. Gulotta, M. Polimeni, S. Lenton, C. G. Starr, A. Stradner, E. Zaccarelli, and P. Schurtenberger. Combining scattering experiments and colloid theory to characterize charge effects in concentrated antibody solutions. *Molecular Pharmaceutics*, 21(5):2250–2271, Apr. 2024.

[11] L. M. Hall, M. J. Stevens, and A. L. Frischknecht. Dynamics of model ionomer melts of various architectures. *Macromolecules*, 45(19):8097–8108, Oct. 2012.

[12] M. K. Hazra and Y. Levy. Charge pattern affects the structure and dynamics of polyampholyte condensates. *Physical Chemistry Chemical Physics*, 22(34):19368–19375, 2020.

[13] H. Hofmann, A. Soranno, A. Borgia, K. Gast, D. Nettels, and B. Schuler. Polymer scaling laws of unfolded and intrinsically disordered proteins quantified with single-molecule spectroscopy. *Proceedings of the National Academy of Sciences*, 109(40):16155–16160, Sept. 2012.

[14] T. Hueckel, G. M. Hocky, J. Palacci, and S. Sacanna. Ionic solids from common colloids. *Nature*, 580(7804):487–490, Apr. 2020.

[15] M. W. Issa, N. R. Baumgartner, M. A. Kalil, S. D. Ryan, and C. L. Wirth. Charged nanoparticles quench the propulsion of active janus colloids. *ACS Omega*, 4(8):13034–13041, Aug. 2019.

[16] R. Kumar, A. H. Slim, A. Faraone, J.-M. Y. Carrillo, R. Poling-Skutvik, M. Muthukumar, A. B. Marciel, and J. C. Conrad. Pivotal roles of triple screening-topological, electrostatic, and hydrodynamic-on dynamics in semidilute polyelectrolyte solutions. *Macromolecules*, 57(6):2888–2896, Mar. 2024.

[17] C. N. Likos. Effective interactions in soft condensed matter physics. *Physics Reports*, 348(4–5):267–439, July 2001.

[18] M. Lund and B. Jönsson. Charge regulation in biomolecular solution. *Quarterly Reviews of Biophysics*, 46(3):265–281, July 2013.

[19] M. Muthukumar. 50th anniversary perspective: A perspective on polyelectrolyte solutions. *Macromolecules*, 50(24):9528–9560, Dec. 2017.

[20] C. Nie, P. Pouyan, D. Lauster, J. Trimpert, Y. Kerkhoff, G. P. Szekeres, M. Wallert, S. Block, A. K. Sahoo, J. Dernedde, K. Pagel, B. B. Kaufer, R. R. Netz, M. Ballauff, and R. Haag. Polysulfates block sars-cov-2 uptake through electrostatic interactions**. *Angewandte Chemie International Edition*, 60(29):15870–15878, June 2021.

[21] S. P. Pineda, R. Staňo, A. Murmiliuk, P. M. Blanco, P. Montes, Z. Tošner, O. Groborz, J. Pánek, M. Hrubý, M. Štěpánek, and P. Košovan. Charge regulation triggers condensation of short oligopeptides to polyelectrolytes. *JACS Au*, 4(5):1775–1785, Mar. 2024.

[22] R. Podgornik. General theory of charge regulation and surface differential capacitance. *The Journal of Chemical Physics*, 149(10), Sept. 2018.

[23] M. Polimeni, E. Zaccarelli, A. Gulotta, M. Lund, A. Stradner, and P. Schurtenberger. A multi-scale numerical approach to study monoclonal antibodies in solution. *APL Bioengineering*, 8(1), Feb. 2024.

[24] N. C. Seeman and H. F. Sleiman. Dna nanotechnology. *Nature Reviews Materials*, 3(1), Nov. 2017.

[25] C. E. Sing and S. L. Perry. Recent progress in the science of complex coacervation. *Soft Matter*, 16(12):2885–2914, 2020.

[26] C. C. M. Sproncken, B. Gumí-Audenis, S. Foroutanparsa, J. R. Magana, and I. K. Voets. Controlling the formation of polyelectrolyte complex nanoparticles using programmable ph reactions. *Macromolecules*, 56(1):226–233, Dec. 2022.

[27] S. Srivastava, A. E. Levi, D. J. Goldfeld, and M. V. Tirrell. Structure, morphology, and rheology of polyelectrolyte complex hydrogels formed by self-assembly of oppositely charged triblock polyelectrolytes. *Macromolecules*, 53(14):5763–5774, July 2020.

[28] R. Staňo, J. Smrek, and C. N. Likos. Cluster formation in solutions of polyelectrolyte rings. *ACS Nano*, 17(21):21369–21382, Sept. 2023.

[29] E. Stiakakis, N. Jung, N. Adžić, T. Balandin, E. Kentzinger, U. Rücker, R. Biehl, J. K. G. Dhont, U. Jonas, and C. N. Likos. Self assembling cluster crystals from dna based dendritic nanostructures. *Nature Communications*, 12(1), Dec. 2021.

[30] A. Stradner and P. Schurtenberger. Potential and limits of a colloid approach to protein solutions. *Soft Matter*, 16(2):307–323, 2020.

[31] W. Tao, J. Wang, W. J. Parak, O. C. Farokhzad, and J. Shi. Nanobuffering of ph-responsive polymers: A known but sometimes overlooked phenomenon and its biological applications. *ACS Nano*, 13(5):4876–4882, Apr. 2019.

[32] M. Tirrell. Polyelectrolyte complexes: Fluid or solid? *ACS Central Science*, 4(5):532–533, May 2018.

[33] I. K. Voets, A. de Keizer, and M. A. Cohen Stuart. Complex coacervate core micelles. *Advances in Colloid and Interface Science*, 147–148:300–318, Mar. 2009.

Schedule

Monday, September 8

12:00 – 14:00	Registration
14:00 – 14:15	Opening & Information for the Participants
	Chair: **Christos N. Likos**
14:15 – 14:45	**Peter Schurtenberger**: Exploring charge effects in soft matter: responsive particles, shape anisotropy and the role of charge patches
14:45 – 15:15	**Ilja Voets**: On Complex(ed) Relations: the Power and Peculiarities of Nanoscopic Polyelectrolyte-based Particles
15:15 – 15:45	**Jeetain Mittal**: Wiggles to Flow: Multiscale Dynamics of Charged Protein Condensates
15:45 – 17:30	Welcome Reception

Tuesday, September 9

	Chair: **Christos N. Likos**
09:00 – 09:30	**David Andelman**: Remembering Rudi Podgornik: Charged liquids, electrified interfaces and more
09:30 – 10:00	**Anže Božič**: Evolutionary changes in charge on spike protein of SARS-CoV-2
10:00 – 10:30	**Nataša Adžić**: Field-theoretic approach to charged Janus colloids beyond mean field
10:30 – 11:00	Coffee Break
	Chair: **Peter Košovan**
11:00 – 11:30	**Andreas Walther**: Phase Separation of DNA: From Fundamentals to Artificial Cells
11:30 – 12:00	**Ronald Larson**: pH and Salt-Dependent Charging and Coacervation of Weak Polyelectrolytes: Hydrophobic Effects
12:00 – 12:30	**Stefanie Schneider**: Monte Carlo Simulations of pH-sensitive polyelectrolyte microgels
12:30 – 14:00	Lunch Break
	Chair: **Roman Staňo**
14:00 – 14:30	**Matthias Ballauff**: Driving Forces in the Formation of Biocondensates of Highly Charged Proteins
14:30 – 15:00	**Hannes Ausserwöger**: Biomolecular condensates sustain pH gradients at equilibrium through charge neutralisation
15:00 – 15:30	Coffee Break
	Chair: **Emanuela Bianchi**
15:30 – 16:00	**Jeffrey Everts**: The interplay between electric double layers and nematic order
16:00 – 16:30	**Vitja Beltram**: Charged Active Nematics

Wednesday, September 10

	Chair: **Stefanie Schneider**
09:00 – 09:30	**Ahmad Reza Motezakker**: Simulation of Structure and Mechanics in Electrostatic Hybrid Networks
09:30 – 10:00	**Tomáš Sedlačík**: Charge in Double-Network Hydrogels: A Key to Understanding Toughening Synergy?
10:00 – 10:30	**Dikla Kolan**: Propagation of a chemo-mechanical phase boundary in polyacrylate gels
10:30 – 11:00	Coffee Break
	Chair: **Emanuela Bianchi**
11:00 – 11:30	**Stefano Sacanna**: Harnessing Coulombic Forces to guide Colloidal Self-assembly
11:30 – 12:00	**Peter van Oostrum**: Harnessing the Triboelectric Effect for Patchy Particles Synthesis: Properties and Self-Assembly
12:00 – 12:30	**Jan Dhont**: Temperature Induced Migration of Interacting Charged Colloidal Particles
12:30 – 14:00	Lunch Break
	Chair: **Peter Košovan**
14:00 – 14:30	**Ulrich Scheler**: Counterion condensation, effective charge and ligand binding on macromolecules studied by PFG NMR
14:30 – 15:00	**Iris Smokers**: Selective ion binding and uptake shape the microenvironment of biomolecular condensates
15:00 – 15:30	**Friederike Schmid**: Self-assembling nanoparticles for medical applications
15:30 – 17:30	Poster Session

Thursday, September 11

	Chair: **Pablo M. Blanco**
09:00 – 09:30	**Daniele Parisi**: Asymmetry in Biopolymer Complex Coacervates: Decoding the Interplay of Molecular Weight, Flexibility, and Ionic Strength
09:30 – 10:00	**Aida Naghilou**: Scanning probe microscopy for elucidating the rheological properties of biomolecular condensates during gelation and rejuvenation
10:00 – 10:30	**Mehdi Vahdati**: Unifying the dynamics of viscoelastic liquids across the complex coacervation phase diagram: time-polyelectrolyte-salt superposition
10:30 – 11:00	Coffee Break
	Chair: **Matthias Ballauff**
11:00 – 11:30	**Fabrizio Camerin**: A Colloidal Framework for Decoding Charge Heterogeneity in Antibody Solutions
11:30 – 12:00	**Sebastian Pineda**: Patchy charge distribution affects the pH in protein solutions during dialysis.
12:00 – 12:30	**Mikael Lund**: Anisotropic Interactions and Intermolecular Pose Exploration using Subdivided Spheres
12:30 – 14:00	Lunch Break
	Chair: **Chara Alexiou**
14:00 – 14:30	**Christos N. Likos**: Polymer topology and charged soft matter: a tale of rings
14:30 – 15:00	**Franco Ferrari**: Some nontrivial thermodynamic properties of polymer catenanes and chainmails in a salt solution
15:00 – 15:30	Coffee Break
	Chair: **Tomáš Sedlačík**
15:30 – 16:00	**Igor Lacík**: Propagation rate coefficient in radical polymerization for charged monomers polymerized in aqueous solutions
16:00 – 16:30	**Morine Nader**: Electroadhesion: Reversibly Adhering Hydrogels to Tissues Using Electric Fields
18:30 – 21:30	Workshop Dinner (Heuriger Feuerwehr Wagner)

Friday, September 12

	Chair: **Hannes Ausserwöger**
09:00 – 09:30	**Marketa Schmidt Cernohorska**: Biomechanical resilience in centrosome kinetics
09:30 – 10:00	**Adam Harmat**: Toward ”phase” diagrams in multidomain protein solutions in vitro
10:00 – 10:30	**Valerio Sorichetti**: Charged for attraction: How biomolecular condensates pull chromosomes together
10:30 – 11:00	Coffee Break
	Chair: **Roman Staňo**
11:00 – 11:30	**Cristian Micheletti**: Nanopore translocation of entangled DNA and RNA filaments
11:30 – 12:00	**Juan Elezgaray**: DNA origamis: their folding process and their interactions with lipid membranes
12:00 – 12:30	**Jennifer Tersteegen**: Diverse non-equilibrium behavior of protein condensates in electric fields
12:30 – 12:45	Closing & Concluding Remarks

Participants

Neda Abbasi	University of Szczecin (Poland)
Nataša Adžić	Institute of Physics Belgrade (Serbia)
Reyhaneh Afghani Farimani	University of Vienna (Austria)
Chara Alexiou	University of Vienna (Austria)
David Andelman	Tel Aviv University (Israel)
Hannes Ausserwöger	University of Cambridge (United Kingdom)
Mathias Ballauff	Free University of Berlin (Germany)
Vitja Beltram	Jožef Štefan Institute Ljubljana (Slovenia)
Emanuela Bianchi	Vienna University of Technology (Austria)
Pablo M. Blanco	Norwegian University of Science and Technology (Norway)
Anže Božič	Jožef Štefan Institute Ljubljana (Slovenia)
Fabrizio Camerin	Lund University (Sweden)
Saikat Chakraborty	Grenoble Alpes University (France)
Gabriel Federico Debais	Aalto University (Finland)
Jan Dhont	Forschungszentrum Jülich (Germany)
Juan Elezgaray	French National Centre for Scientific Research Bordeaux (France)
Jeffrey Everts	University of Warsaw (Poland)
Franco Ferrari	University of Szczecin (Poland)
Steph Flores	University of Manchester (United Kingdom)
Francesca Galluzzi	Foundation for Research and Technology-Hellas (Greece)
Adam Harmat	Aalto University (Finland)
Panagiotis Ilia	The Cyprus Institute (Cyprus)
Vojtěch Keprta	Charles University (Czechia)
Dikla Kolan	University of Haifa (Israel)
Peter Košovan	Charles University (Czechia)
Igor Lacík	Slovak Academy of Sciences (Slovakia)
Ronald Larson	University of Michigan (United States)
Christos N. Likos	University of Vienna (Austria)
Mikael Lund	Lund University (Sweden)
Theodora Menidiati	Forschungszentrum Jülich (Germany)
Cristian Micheletti	International School for Advanced Studies (Italy)
Jeetain Mittal	Texas A&M University (United States)
Ahmad Reza Motezakker	KTH Royal Institute of Technology (Sweden)
Morine Nader	University of Maryland (United States)
Aida Naghilou	Medical University of Vienna (Austria)
Miroslava Nedyalkova	University Fribourg (Switzerland)
Ipsita Padhee	Charles University (Czechia)
Daniele Parisi	University of Groningen (Netherlands)
Sebastian Pineda	Charles University (Czechia)
Stefano Sacanna	New York University (United States)
Ulrich Scheler	Leibniz Institute of Polymer Research Dresden (Germany)
Friederike Schmid	Johannes Gutenberg University Mainz (Germany)
Marketa Schmidt Cernohorska	Jan Evangelista Purkyně University in Ústí nad Labem (Czechia)
Stephanie Schneider	RWTH Aachen University (Germany)
Peter Schurtenberger	Lund University (Sweden)
Tomáš Sedlačík	University of Chemistry and Technology, Prague (Czechia)
Amir Sheikh Shoaei	Dresden University of Technology (Germany)
Iris Smokers	Radboud University (Netherlands)
Valerio Sorichetti	Institute of Science and Technology Austria (Austria)
Eliška Stančíková	Charles University (Czechia)
Roman Staňo	University of Cambridge (United Kingdom)
Anna Stradner	Lund University (Sweden)
Andrea Tagliabue	University of Genoa (Italy)
Jennifer Tersteegen	Aalto University (Finland)
Mehdi Vahdati	Institute Charles Sadron (France)
Peter van Oostrum	University of Natural Resources and Life Sciences, Vienna (Austria)
Ilja Voets	Eindhoven University of Technology (Netherlands)
Fran Ivan Vrban	University of Ljubljana (Slovenia)
Andreas Walther	Johannes Gutenberg University Mainz (Germany)
Takahiro Yokoyama	Leibniz Institute of Polymer Research Dresden (Germany)

Talks

Field-theoretic approach to charged Janus colloids beyond mean field

Nataša Adžić (Institute of Physics Belgrade)

The self-assembly of charged biological entities is a topic of fundamental importance in both fundamental and applied sciences. Our current understanding of how uniformly charged particles, ranging from the nano- to micron-scale, interact in polar solvents with dissolved salts largely relies on the mean-field framework, i.e. DLVO theory. While recent extensions of DLVO-like models have incorporated particles with non-uniform charge distributions, their applicability remains limited primarily to conditions involving higher concentrations of monovalent salts.

This talk aims to address the self-assembly behavior of anisotropically charged colloids in solutions that also contain polyvalent ions. It is well established that the strong coupling between polyvalent salts and macroions can give rise to unusual electrostatic phenomena, such as like-charge attraction. However, the impact of these interactions on the phase behavior of anisotropically charged colloidal suspensions remains poorly understood.

To tackle this complex problem, we begin with a simplified model of charged Janus colloids immersed in an asymmetric ionic environment. By employing a field-theoretic approach, we derive the effective electrostatic interactions, which can then be incorporated into coarse-grained models suitable for simulation studies.

Remembering Rudi Podgornik: Charged liquids, electrified interfaces and more

David Andelman (Tel Aviv University)

The purpose of this talk is twofold. First, to highlight the significant contributions of the late Professor Rudolf Podgornik in five research areas: physics of DNA, virus capsids, Casimir effect, fluctuation-induced interactions, and the role of electric charge in soft matter systems. Second, to introduce two projects related to charged soft matter. (i) The surface tension of electrolytes has a history spanning a century, beginning with Onsager's groundbreaking work. This topic will be examined again using a field-theoretical approach that incorporates ionic specificity based on the Hofmeister series. (ii) The idea of charge regulation provides a more realistic way to understand biomolecules with charges that can dissociate into the surrounding water. Recent modeling of charge regulation will be presented, along with its applications to proteins, polyelectrolytes, and membranes.

Biomolecular condensates sustain pH gradients at equilibrium through charge neutralisation

Hannes Ausserwöger (University of Cambridge)

Electrochemical gradients are essential to the functioning of cells and form across membranes using active transporters. Here, we show in contrast that condensed biomolecular systems sustain significant pH gradients without any external energy input. By studying individual condensed droplets on the micron scale using a microdroplet platform, we reveal dense phase pH shifts towards conditions of minimal electrostatic repulsion. We demonstrate that by doing so protein condensates can drive substantial alkaline and acidic gradients which are compositionally tuneable and can extend to complex architectures sustaining multiple unique pH conditions simultaneously. Through in silico characterisation of human proteomic condensate networks, we further highlight potential wide ranging electrochemical properties emerging from condensation in nature, while correlating intracellular condensate pH gradients with complex biomolecular composition. Together, the emergent nature of condensation shapes distinct pH microenvironments, thereby creating a unique regulatory mechanism to modulate biochemical activity in living systems.

Driving Forces in the Formation of Biocondensates of Highly Charged Proteins

Matthias Ballauff (Free University of Berlin)

We discuss a general thermodynamic analysis of the complex formation between proteins and polyelectrolytes. This analysis allows us to quantify the main driving forces, namely counterion release and hydration.[1] In particular, the analysis of hydration effects leads to a quantitative understanding of the Hofmeister-effects on the interaction of polyelectrolytes with proteins.[2] In my talk I will discuss this model and its application to biocondensates, that is, the phase separation in mixtures of proteins of opposite charge. In particular, I will present the analysis of the binary complex formation of the highly positively charged linker histone H1 and the highly negatively charged chaperone, prothymosin α (ProTα). ProTα and H1 have large opposite net charges (–44 and +53, respectively) and form complexes at physiological salt concentrations with high affinity as shown by Chowdhury et al.[3] The analysis demonstrates that the release of the counterions mainly bound to ProTα is the main driving force, hydration effects related to water release play no role within the limits of error. A strongly negative Dcp (= -0.87 kJ/(K mol)) is found which is due to the loss of conformational degrees of freedom.[4] The entire analysis demonstrates the basic importance of charge-charge interaction in biologically relevant systems.

References:

[1] J. J. Walkowiak, M. Ballauff, Adv Sci 2021, 8, 2100661.

[2] W. Malicka, R. Haag, M. Ballauff, J Phys Chem B 2022, 126, 6250-6260.

[3] A. Chowdhury, A. Borgia, S. Ghosh, A. Sottini, S. Mitra, R. S. Eapen, M. B. Borgia, T. Yang, N. Galvanetto, M. T. Ivanovic, P. Lukijanczuk, R. Zhu, D. Nettels, A. Kundagrami, B. Schuler, Proc Natl Acad Sci U S A 2023, 120, e2304036120.

[4] M. Ballauff, Biomolecules 2024, 14.

Charged Active Nematics

Vitja Beltram (Jožef Štefan Institute Ljubljana)

A significant focus in the study of isotropic fluids with ions (electrolytes) is placed on charge control, as it plays a key role in the properties of various systems. A common feature is that charge is controlled through surfaces formed between different fluids or between a fluid and a solid. However, setting up these surfaces is not trivial, which can lead to certain limitations in charge control. Compared to isotropic fluids, liquid crystals offer more possibilities for charge control due to their higher degree of order. Charge can be localized in the topological defects of the orientational order.

To better understand various electrostatic effects, including ions, on the dynamics of active complex nematic fluids, we investigated the influence of flexoelectricity and ion partitioning on ion-doped 2D active nematic liquid crystals through numerical simulations and theoretical analysis. First, we studied ion current and magnetic field distribution around single topological defects in active nematics, and then we also examined the role of ions in active turbulence, showing how ion-doped active nematics can generate voltage through variations in magnetic flux induced by moving topological defects.

Evolutionary changes in charge on spike protein of SARS-CoV-2

Anže Božič (Jožef Štefan Institute Ljubljana)

The COVID-19 pandemic offered an unprecedented glimpse into the evolution of its causative virus, SARS-CoV-2. It has been estimated that since its outbreak in late 2019, the virus has explored all possible alternatives in terms of missense mutations for all sites of its polypeptide chain. Spike protein of the virus exhibits the largest sequence variation in particular, with many individual mutations impacting target recognition, cellular entry, and endosomal escape of the virus. Among these, changes to charged amino acid residues have been shown to influence spike protein binding to different cell surface receptors, its non-specific electrostatic interactions with the environment, and its structural stability and conformation. Moreover, recent studies unveiled a significant increase in the total amount of positive charge on the spike protein during SARS-CoV-2 evolution, especially in the initial period of the pandemic.

We have performed a detailed analysis of changes in dissociable amino acids of more than 2600 different SARS-CoV-2 lineages, offering a detailed look into the evolutionary patterns of change of the spike protein charge. Our results show that the previously observed trend toward an increase in the positive charge has essentially stopped with the emergence of the early omicron variants. We also demonstrate that the patterns of change in the number of ionizable amino acids on the spike protein are characteristic of related lineages within the broader clade division of the SARS-CoV-2 phylogenetic tree. What is more, we show that the spike protein exhibits a prominent preference for lysine residues over arginine residues, the ratio of which increased at several points during spike protein evolution, most recently with BA.2.86 and its sublineages. The increased ratio is a consequence of mutations in different structural regions of the spike protein and is now among the highest among viral species in the *Coronaviridae* family. Overall, our work sheds light on the evolutionary changes in the number of dissociable amino acids on the spike protein of SARS-CoV-2, complementing existing studies and providing a stepping stone towards a better understanding of the relationship between the spike protein charge and viral infectivity and transmissibility.

A Colloidal Framework for Decoding Charge Heterogeneity in Antibody Solutions

Fabrizio Camerin (Lund University)

Electrostatics shape the structure, stability, and dynamics of charged (bio)matter, yet how heterogeneous, anisotropic charge distributions control protein–protein interactions remains unclear. I will present a versatile multiscale framework that links molecular electrostatics to collective properties by combining a colloid-inspired coarse-grained model with neural-network–assisted optimization trained against experimental SAXS data.

Using monoclonal antibodies as a representative anisotropic system, the approach identifies coarse-grained charge patterns that reproduce measured structure factors and predict rheological behavior over a wide range of concentrations. Feature-attribution analysis further reveals which physical descriptors and spatial arrangements of localized charge patches dominate the emergent solution structure.

The resulting, transferable strategy offers a predictive route to decipher charge-driven interactions in anisotropic biomolecules and, more broadly, heterogeneously charged soft-matter systems, with immediate relevance to protein formulation and functional materials design.

Temperature Induced Migration of Interacting Charged Colloidal Particles

Jan Dhont (Forschungszentrum Jülich)

The migration of particles induced by spatial gradients in temperature is commonly referred to as thermophoresis, thermodiffusion, thermal diffusion, or the (Ludwig-)Soret effect. The force on colloidal particles that drives such migration depends on the response of single particles and their interactions to variations of temperature. A distinction can thus be made between single-particle and collective contributions to the thermophoretic force experienced by a colloidal particle. There is as yet no systematic theory for thermophoresis of charged colloids that accounts for the collective contribution due to interactions between charged colloids. In a previous study, we developed an irreversible thermodynamics approach for uncharged colloids [Coll. Int. Sci. **666** (2024) 457]. In this presentation this approach is extended to account for electrostatic interactions between charged colloids. Enslavement of ion fluxes to the relatively slowly evolving concentration profile of the colloids, and an approximate evaluation of the heat-of-transfer, leads to microscopic, particle-based expressions for the thermodiffusion coefficient and the Soret coefficient. In addition, an explicit expression for the macroscopic thermoelectric field is derived, which gives rise to a thermoelectrophoretic force. A comparison to existing experimental thermophoresis experiments will presented.

DNA origamis: their folding process and their interactions with lipid membranes

Juan Elezgaray (French National Centre for Scientific Research Bordeaux)

DNA nanotechnology dwelves on the self-assembly properties of nucleic acids for the design of molecular devices, including motors and logic circuits. In particular, DNA origamis are the result of an annealing process, where a long single stranded DNA interacts with a set of short DNA sequences, to yield a well defined structure. Despite the maturity of the field, fundamental questions remain open. In this talk, I will address two of them. First, is the result of the folding process unique? Or under which conditions does the annealing process lead to unwanted structures? Second, DNA origamis can be easily modified with hydrophobic moieties to interact with lipid bilayers, The result of this interaction can be a water channel with a well defined structure. I will discuss how this process can be accelerated in the presence of an external (weak) electric field.

The interplay between electric double layers and nematic order

Jeffrey Everts (University of Warsaw)

Nematic liquid crystals can flow like ordinary liquids, but there are also differences, such as the emergence of elasticity. Nematics can be seen as orientationally ordered anisotropic dielectrics that are flexoelectric - they can form a spontaneous polarisation upon straining the material which is not accounted for in the dielectric tensor. When convoluted with ionic degrees of freedom, several interesting phenomena can occur. I will demonstrate that nematic electrolytes in some cases can be characterized by an anisotropic Debye screening length and how topological defects can become charged and/or cause ionic charge separation around them forming ionic multilayers (instead of the familiar double layers). Furthermore, the topological defects can alter the surface charge distribution of mesoscopic objects such as flat plates or spheres. Finally, I will discuss our work on the charge dynamics of a nematic electrolyte, which in a sense have many similarities with that of an Archimedes' screw: a hydraulic machine that can either pump or generate energy as a turbine. This leads to a coupling of the charge current to the winding density of a liquid crystal, which naturally leads to topological defects being driven by ionic current or being used as inductors.

References:

M. Ravnik and J. C. Everts, *Topological-defect-induced surface charge heterogeneities in nematic electrolytes*, Phys. Rev. Lett. **125**, 037801 (2020).

J. C. Everts and M. Ravnik, *Charge-, salt- and flexoelectricity-driven anchoring effects in nematics*, Liq. Cryst. **48**, 423 (2021).

J. C. Everts*, B. Senyuk*, H. Mundoor, M. Ravnik and I. I. Smalyukh, *Anisotropic electrostatic screening of charged colloids in nematic solvents*, Sci. Adv. **7**, eabd0662 (2021).

J. C. Everts and M. Ravnik, *Ionically charged topological defects in nematic fluids*, Phys. Rev. X **11**, 011054 (2021).

C. Dao, J. C. Everts, M. Ravnik, and Y. Tserkovnyak, *Nematronics: Reciprocal coupling between ionic currents and nematic dynamics*, Phys. Rev. Lett. **130**, 168102 (2023).

Some nontrivial thermodynamic properties of polymer catenanes and chainmails in a salt solution

Franco Ferrari (University of Szczecin)

Charged diblock copolymer rings linked together and fluctuating in an ion solution that screens the long range Coulomb interactions are considered. The thermodynamic properties of the circular polymer catenanes of L.Tubiana et al, PRL 129 (2022), 227801, are discussed. It is found that these catenanes have a few phase transitions. Two of them have been identified and correspond to the different scales which are relevant for the circular catenane: that of the single rings and that of the catenane as a whole. Finally, the results of the simulations of simple chainmails composed of a maximum of forty rings will be presented.

Toward "phase" diagrams in multidomain protein solutions in vitro

Adam Harmat (Aalto University)

Phase transitions are ubiquitous in nature, taking part in the formation of both synthetic and living materials. In cells, biomolecule solutions can undergo liquid-liquid phase separation but also various liquid to solid-like transitions (i.e. aggregation and gelation) that regulate biochemical processes. Uncovering the assembly phase behavior of one-component protein solutions *in vitro* is the first step toward understanding the non-equilibrium behavior of multicomponent solutions in living organisms. Globular and intrinsically disordered protein solutions are relatively well understood and conceptualized via colloidal and polymer theories that highlight the role of electrostatic interactions. However, solutions of multidomain proteins containing both folded and intrinsically disordered regions (IDRs) are less studied.

To fill this gap, we investigate the assembly phase behavior of an *in vitro* solution of an engineered recombinant silk-like protein, NT-2Rep-CT, containing two folded terminal domains connected by an IDR tether. We showed by light microscopy and analytical ultracentrifugation measurements that the protein solution can exist in multiple material states including homogenous dilute solutions, metastable liquid-liquid coexistence, and irreversible aggregates. The experiments highlight the challenge in identifying equilibrium states but also demonstrate the critical role of metastability of the solution and its aging on the properties of the final material. To understand and generalize the findings, we have considered the thermodynamics of the system and proposed a minimalist phase diagram for the assembly phase response of the NT-2Rep-CT protein. The work paves way toward a generalized understanding of in vitro protein solutions.

References:

[1] Fedorov, Escalona, Tolmachev, Harmat, Scacchi, Sammalkorpi, Aranko, Linder, *Small* 20 2306817 (2024).

[2] Fedorov*, Sammalisto*, Harmat*, Ahlberg, Koskela, Haataja, Scacchi, Sammalkorpi, Linder, *Advanced Functional Materials* 35 2410421 (2025).

Propagation of a chemo-mechanical phase boundary in polyacrylate gels

Dikla Kolan (University of Haifa)

The competition between mono- and divalent counterions in polyelectrolyte gels can lead to reversible transitions between swollen and collapsed phases. In this study, we investigate the emergence of a propagating boundary that separates the two phases in cylindrical polyacrylate gels, where it moves along the gel's longitudinal axis. We emphasize the distinction between an overall calcium-induced contraction and the axial progression phenomenon and use an object detection algorithm to determine the boundary propagation rate. Additionally, we investigate how calcium concentration, external voltage, and gel diameter influence the formation time and propagation velocity of the phase boundary. Our findings reveal that an increased calcium concentration in the adjacent bath, the application of an external voltage, and a decreased gel diameter contribute to a shorter formation time and a higher propagation velocity of the phase boundary. These results provide important insights into the complex dynamics of phase boundaries in cylindrical polyelectrolyte gels.

Propagation rate coefficient in radical polymerization for charged monomers polymerized in aqueous solutions

Igor Lacík (Slovak Academy of Sciences)

The central goal of this contribution is to introduce to the attendees of the workshop *Charged Soft Matter: Bridging Theory and Experiment* the topic of radical polymerization in aqueous solutions, particularly the issues connected with the propagation rate coefficient, $k\mathrm{p}$, for charged monomers. The $k\mathrm{p}$ values are of principal interest for understanding of radical polymerization, simply because they determine the rate of polymer chain growth, i.e. the polymer formation by addition of unsaturated monomer to the growing radical chain-end. Additionally, they are required to determine termination and transfer rate coefficients to ultimately enable modeling of polymerization kinetics and molar mass of resulting polymers. This principle genuinely requires the access to accurate kp values, which became available to the polymer community thanks to the pioneering work of Prof. O.-F. Olaj and his co-workers from the University of Vienna, who introduced the combination of pulsed-laser polymerization with size-exclusion chromatography (PLP-SEC) as a straightforward method for kp determination [1].

The kp values determined for a given monomer in different solvents provide the information on the effect of the solvent environment on the propagation step. This phenomenon is known as a solvent effect that is specifically manifested for polymerizations carried out in aqueous solutions. The presence of functional groups (e.g., hydroxy, carboxy, amino, ammonium, carboxylate, sulfate) in the monomer structure gives rise to intra and intermolecular specific interactions (hydrogen bonding, electrostatic, van der Waals) that are amplified by interactions with water used as a solvent. This greatly complicates the understanding of the polymerization mechanism and kinetics compared to the polymerizations in non-aqueous solutions. In the last two decades we achieved a significant understanding of radical polymerization for water-soluble monomers in aqueous solutions, with the comprehensive summary recently published by Buback et al [2]. For different monomer categories, the dependence of kp values on monomer concentration, monomer conversion, temperature, pressure, and for ionized and ionizable monomers, on degree of ionization and ionic strength became available along with understanding of fundamental mechanisms determining the magnitude of kp values. The mechanistic picture of chain growth, already challenging for non-ionized monomers due to the presence of predominantly hydrogen bonding interactions, is further complicated by the presence of electrostatic interactions in the case of charged monomers. The kp values were determined for ionized acrylic [3] and methacrylic [4] acids, zwiterionic monomers [5], and cationic monomers [6].

Our work focusing on the determination of the kp values for fully charged monomers by using the PLP-SEC method will be presented in more detail. The effect of polymerization conditions, including monomer concentration, concentration of added salt, temperature, pH, will be shown for cationically charged monomers [2-(methacryloyloxyl)ethyl]trimethylammonium chloride (TMAEMC) and [3-(methacryloylamino)propyl] trimethyl ammonium chloride (MAPTAC), cationically ionizable 2-(dimethylamino)ethyl methacrylate (DMAEMA), and for anionically charged sodium methacrylate (MAANa). The propagation step is governed by the molar concentration of counterions that are introduced to the polymerization system. At very low counterion content, repulsive electrostatic interactions dominate. Upon sufficient screening of these interactions by counterions, the kp values follow the trends seen for non-ionized monomers. A linear correlation between kp values and the molar concentration of counterions was found for polymerization of TMAEMC and MAPTAC. The comparison between kp for TMAEMC and MAPTAC monomers vs MAANa points at the importance of the spacer length between the charged group and the C=C double bond of a monomer. This spacer is shorter for MAANa than for TMAEMC and MAPTAC, which corresponds to higher repulsive interactions requiring a higher counterion content for effective screening in the case of MAANa than of TMAEMC and MAPTAC. These and other findings will be reported to present the current understanding of radical polymerization for charged monomers in aqueous solutions and the effect of polymerization conditions on kp values.

References:

[1] Olaj, O.F., Bitai, I., Hinkelmann, F. *Makromol. Chem.* 1987, 188, 1689.

[2] Buback, M., Hutchinson, R. A., Lacík, I. *Prog. Polym. Sci.* 2023, 138, 101645.

[3] Lacík, I., Beuermann, S., Buback, M. *Macromol. Chem. Phys.* 2004, 205, 1080.

[4] Lacík, I., Učňová, L., Kukučková, S., Buback, M., Hesse, P., Beuermann S. *Macromolecules* 2009, 42, 7753.

[5] Lacík, I., Sobolčiak, P., Stach, M., Chorvát, D., Kasák P. *Polymer* 2016, 87, 38.

[6] Urbanová, A., Ezenwajiaku, I. H., Nikitin, A.N., Sedlák, M., Vale, H.M., Hutchinson, R.A.H., Lacík, I. *Macromolecules* 2021, 54, 3204.

Acknowledgement. This work was supported by the Slovak Scientific Grant Agency VEGA 2/0143/23 and by funding from BASF SE Ludwighshafen, Germany.

pH and Salt-Dependent Charging and Coacervation of Weak Polyelectrolytes: Hydrophobic Effects

Ronald Larson (University of Michigan)

By treating deprotonation and cation binding in polyacids as reversible reactions and using a random phase approximation (RPA) that captures the chain connectivity, the pH-dependent ionization of acid groups along a polyacid chain is predicted and compared with results of experiments for titration of rodlike and Gaussian coil polyacids. We find that the former is followed by hydrophilic poly(acrylic acid) (PAA), while the latter is followed more closely by hydrophobic poly(2-acrylamido-2-methyl-1-propanesulfonic acid). Large deviations from Henderson-Hasselbalch behavior are both observed and successfully predicted by the theory. We also investigate PAA hydrophobicity through its phase separation from solutions of water and polyelectrolyte, which we model by a Flory chi parameters. Finally, we measure and model the phase behavior of mixtures of poly(acrylic acid) (PAA) and poly(diallyldimethylammonium), PDADMA in both NaCl and KCl salts at pH values ranging from 4.9 to 7.0, where the PAA ranges from partially to fully charged. We find significant and unexpected changes in phase behavior as a function of salt concentration and pH, showing strong effects of hydrophobicity of PAA in both the charge regulation and phase behavior. The phase behavior can be qualitatively predicted by theory, with parameters in part predicted by molecular dynamics simulations.

Polymer topology and charged soft matter: a tale of rings

Christos Likos (University of Vienna)

Ring polymer solutions feature distinct rheological properties stemming from the unique forms of self-organization and mutual entanglements that have their roots on the circular topology of these macromolecules. Although quite a bit is known about melts of long and flexible ring polymers, the Physics of short minirings whose persistence length is comparable to their contour size is much less known. In addition, the role of electric charge along the rings' backbone is poorly understood to-date. In this talk, I will present recent results on the interplay between polymer topology and (tunable) electric charge: in the first instance, it will be shown that concentrated solutions of semiflexible ring-shaped polyelectrolytes form a particular kind of cluster glass, in which rheology can be tuned by the concentration and valency of the counterions, whereby multivalent counterions act as glue that stiffens the glass but monovalent counterions melt it [1]. In the second instance, we will consider ribbon-shapled rings and we will demonstrate that changing the pH of the solution leads to a local tuing of the twist/writhe balance along the backbone, resulting into the formation of charge-regulated coexsitence between writhe-rich and twist-rich domains along the polymer backbone [2].

References:

[1] Roman Stano, Jan Smrek, and Christos N. Likos, **Cluster formation in solutions of polyelectrolyte rings**, ACS Nano **17**, 21369 - 21382 (2023).

[2] Roman Stano, Christos N. Likos, Davide Michieletto, and Jan Smrek, **Topology-controlled microphase separation and interconversion of twist and writhe domains in supecoiled annealed polyelectrolytes**, Physical Review Letters **135**, 048101 (2025).

Anisotropic Interactions and Intermolecular Pose Exploration using Subdivided Spheres

Mikael Lund (Lund University)

Understanding interactions between large, aspherical macromolecules such as proteins and colloids require careful consideration of angular dependent forces. Surface charge anisotropy, for example, leads to a surprising non-monotonic ionic strength dependence of measured osmotic second virial coefficient for globular proteins. We review a number of recent experimental and computational findings where intermolecular anisotropy is manifested. To fully bridge theory and experiment, large-scale computer simulations of many macromolecules are often needed. Exploring the vast configurational space is however computationally intensive and large speedups can be gained with high-dimensional lookup tables. We present a new approach to such tables using *subdivided spheres* in order to construct 6D tables, storing angular dependent energies between protein pairs. In addition to offering convenient interpolation, the tables have the unintended, but pleasant property that they allows for explicit evaluation of the configurational integral and derived twobody thermodynamics. We use this to explore protein osmotic virial coefficients using the recent Calvados coarse grained model and light-scattering experiments. Software for calculating virial coefficients and potential of mean force is available at `https://github.com/mlund/duello`.

Nanopore translocation of entangled DNA and RNA filaments

Cristian Micheletti (International School for Advanced Studies)

Polymer translocation, the process of pulling single filamentous molecules through narrow pores, has long been studied as an example of out-of-equilibrium statistical mechanics and for its relevance in DNA sequencing and biological processes. However, the case in which the polymer structure itself is deeply altered by translocation remains largely unexplored. Here, we address this phenomenon in two contexts involving nucleic acid filaments. First, we discuss DNA unzipping, where one of the two strands is pulled through a nanopore, while the other remains outside [1,2]. Next, we will extend considerations to xrRNAs, short and highly pseudoknotted RNAs that can withstand degradation by exonucleases. We use native-centric atomistic models and translocation simulations to elucidate the mechanistic basis of xrRNA resistance to degradation, demonstrating its dependence on the entangled architecture of xrRNA [3,4]. Finally, we will discuss recent results on the pore translocation of long DNAs, where experiments and simulations indicate that the torque imparted by the solvent flow induces the formation of plectonemes [5].

References:

[1] A. Suma, V. Carnevale and C. Micheletti, ”Nonequilibrium thermodynamics of DNA nanopore unzipping”, Phys. Rev. Lett., (2023), 130 048101

[2] A. Suma and C. Micheletti, ”Unzipping of knotted DNA via nanopore translocation”, QRB Discovery 6 (2025) e4

[3] M. Becchi, P. Chiarantoni and C. Micheletti, RNA Pore Translocation with Static and Periodic Forces: Effect of Secondary and Tertiary Elements on Process Activation and Duration, J. Phys. Chem. B, 125, 1098-1196 (2021)

[4] M. Becchi, P. Chiarantoni and C. Micheletti ”RNA Pore Translocation with Static and Periodic Forces: Effect of Secondary and Tertiary Elements on Process Activation and Duration”, J. Phys. Chem. B, 125, 1098-1196 (2021)

[5] F. Zheng, A. Suma, C. Maffeo, K. Chen, M. Alawami, J. Sha, A. Aksimentiev, C. Micheletti, and U.F. Keyser, ”Torsion-driven plectoneme formation during nanopore translocation of DNA polymers”, Phys. Rev. X art. no. 023116(2025)

From Wiggles to Flow: Multiscale Dynamics of Charged Protein Condensates

Jeetain Mittal (Texas A&M University)

Intrinsically disordered proteins (IDPs) can undergo liquid–liquid phase separation and coacervation, producing biomolecular condensates with diverse structural and rheological properties. The interplay between sequence-dependent electrostatic interactions and conformational heterogeneity gives rise to complex behavior spanning molecular to macroscopic scales. In this talk, I will present recent advances from my group that integrate physics-based simulations with experimental measurements to reveal how molecular driving forces shape condensate structure, dynamics, and material response. Our recent study demonstrated that dilute-phase conformations are predictive of condensate mechanics, providing a framework for connecting single-chain behavior to bulk properties1. Building on this, our latest work extends to understanding internal condensate dynamics across length and time scales, revealing how local motions and interactions contribute to emergent macroscopic behavior2. Together, these results offer a multiscale picture linking microscopic organization and interactions to macroscopic flow and relaxation, with implications for both natural biological assemblies and engineered soft materials.

References:

[1] Sundaravadivelu Devarajan, D., Wang, J., Szała-Mendyk, B., Rekhi, S., Nikoubashman, A., Kim, Y. C., & Mittal, J. (2024). Sequence-dependent material properties of biomolecular condensates and their relation to dilute phase conformations. *Nature Communications*, 15(1), 1912.

[2] Muthukumar, K., Devarajan, D. S., Kim, Y. C., & Mittal, J. (2025). Sticky Interactions Govern Sequence-Dependent Dynamics in Biomolecular Condensates. *bioRxiv*, 2025-07.

Simulation of Structure and Mechanics in Electrostatic Hybrid Networks

Ahmad Reza Motezakker (KTH Royal Institute of Technology)

Soft matter systems held together by electrostatic interactions exhibit a rich spectrum of structures and mechanical behaviors. Using coarse-grained simulations, we examine how variations in composition and interaction parameters drive the evolution of these systems from dispersed constituents to interconnected networks. The study identifies distinct structural regimes and links them to changes in particle dynamics and mechanical response. These findings provide general insights into the relationship between nanoscale organization and bulk properties in electrostatically assembled soft materials.

Electroadhesion: Reversibly Adhering Hydrogels to Tissues Using Electric Fields

Morine Nader (University of Maryland)

We describe the phenomenon of *electroadhesion* (EA) i.e., adhesion that can be switched on by an electric field. EA is induced between a pair of cationic and anionic materials due to electrophoresis of chain segments across the interface. Typically, we fix the cationic material to be a covalently crosslinked hydrogel made by polymerizing cationic monomers. The anionic material could be another gel, or more interestingly, it could be a biological tissue. We have discovered that cationic gels can be adhered by EA to *tissues across all of biology.* This includes tissues from animals, including humans and other mammals, birds, fish, reptiles, etc. Gels can also be adhered to soft tissues from plants, including fruits and vegetables. In all cases, EA is induced by a low electric field (DC, 10 V) applied for a short time (20 s). After the field is removed, the adhesion is permanent. The adhesion can also be reversed by applying the field with opposite polarity. The higher the concentration of anionic polymers in a tissue, the stronger its adhesion to cationic gels. One potential application of EA is in sutureless surgery, i.e., to seal cuts or tears in tissues by adhereing a gel patch over the injured tissue. Preliminary studies with mice show that surgeries can indeed be performed safely and effectively using EA.

References:

[1] L. K. Borden, A. Gargava, S. R. Raghavan. *Reversible electroadhesion of hydrogels to animal tissues for suture-less repair of cuts or tears.* **Nature Communications**, 2021, 12, 4419.

[2] L. K. Borden, A. Gargava, U. J. Kokilepersaud, S. R. Raghavan. *Universal way to "glue" capsules and gels into 3D structures by electroadhesion.* **ACS Applied Materials & Interfaces**, 2023, 15, 20014.

[3] L. K. Borden, M. G. Nader, F. A. Burni, S. M. Grasso, I. Orueta-Ortega, M. Srivastava, P. Montero-Atienza, M. Erdi, S. L. Wright, R. Sarkar, A. D. Sandler, S. R. Raghavan. *Switchable adhesion of hydrogels to plant and animal tissues.* **Advanced Science**, 2025, 12, 2411942.

Scanning probe microscopy for elucidating the rheological properties of biomolecular condensates during gelation and rejuvenation

Aida Naghilou (Medical University of Vienna)

A comprehensive understanding of the dynamics and solidification of biomolecular condensates is closely tied to analysis of their mechanical characteristics [1]. Despite recent technical advances in rheological studies of condensates, these still vastly rely on methods restricted to small forces, rendering measurements of droplets with higher elasticities and after transition to solids challenging. In this work [2, 3], we develop assays for in-depth mechanical characterization of biomolecular condensates by scanning probe microscopy. We demonstrate this technique by measuring the rheological behavior of heterotypic poly-L-lysine heparin condensates, showcasing their multi-route transition from liquid-like to gel as well as their rejuvenation by chemical alterations of the medium. Due to the widespread application of scanning probe microscopy in biological fields, its capability for rapid, high-throughput, high-force range studies, and integration with nanoscale morphological measurements, our probe-based method is a significant step toward advancing the understanding of condensate behavior, leading to accelerated development of therapies.

References:

[1] L. Jawerth, E. Fischer-Friedrich, S. Saha, J. Wang, T. Franzmann, X. Zhang, J. Sachweh, M. Ruer, M. Ijavi, S. Saha, J. Mahamid, A.A. Hyman, F. Jülicher, Protein condensates as aging Maxwell fluids, Science, 370 (2020) 1317-1323.

[2] A. Naghilou, O. Armbruster, A. Mashaghi, , Scanning probe microscopy elucidates gelation and rejuvenation of biomolecular condensates, Cell Reports Physical Science, 6 (2025).

[3] A. Naghilou, T.M.J. Evers, O. Armbruster, V. Satarifard, A. Mashaghi, Synthesis and characterization of phase-separated extracellular condensates in interactions with cells, Chemical Engineering Journal, 518 (2025) 164551.

Asymmetry in Biopolymer Complex Coacervates: Decoding the Interplay of Molecular Weight, Flexibility, and Ionic Strength

Daniele Parisi (University of Groningen)

Complex coacervates formed from oppositely charged biopolymers offer a powerful platform for tunable soft materials with applications ranging from underwater adhesives to biomedical scaffolds. While the effects of polymer chemistry and ionic conditions on coacervate dynamics are well documented, the role of **molecular asymmetry**, particularly in **molecular weight and chain flexibility** remains underexplored. In this study, we investigate the salt-dependent viscoelasticity and adhesion of **hyaluronic acid (HA)–chitosan (CHI)** coacervates, focusing on how symmetry or asymmetry in polymer molecular weight and rigidity affects network formation and mechanical performance. We constructed a library of nine HA–CHI coacervate systems varying systematically in polymer molecular weight combinations, spanning both symmetric (matched Mw) and asymmetric (mismatched Mw) pairs. Using **small-amplitude oscillatory shear (SAOS)** rheology, **van Gurp–Palmen plots**, and **probe tack adhesion testing**, we mapped the influence of salt concentration (0–0.8 M NaCl) on dynamic relaxation, plateau modulus, and adhesive strength. Our results reveal a clear distinction between **unentangled** and **entangled** coacervates. Unentangled systems, such as low-MW HA/CHI pairs, display rapid terminal relaxation and obey **time-salt superposition (tSS)** across a wide frequency window, consistent with models of electrostatically governed relaxation. In contrast, entangled systems exhibit **non-universal scaling** due to salt-insensitive relaxation mechanisms like chain retraction, hydration shell effects, and topological constraints – particularly pronounced in coacervates with high-MW HA. Interestingly, molecular asymmetry plays a critical role: coacervates with **flexible, high-MW CHI** and shorter HA chains exhibit strong adhesion and dynamic responsiveness at low salt, but rapidly lose cohesion with increasing ionic strength. In contrast, systems dominated by **rigid, high-MW HA** maintain mechanical resilience and slower dynamics even under salt stress, though at the cost of reduced interfacial adhesion. Together, these findings provide new insights into the **structure-dynamics-adhesion relationship** in charged polymer networks and highlight how **asymmetric combinations of chain length and flexibility** can be strategically used to balance salt responsiveness and mechanical performance. These principles open new pathways for designing bioinspired coacervates for **adhesives, drug delivery, and soft tissue engineering**.

Patchy charge distribution affects the pH in protein solutions during dialysis

Sebastian Pineda Pineda (Charles University)

When using dialysis or ultra/diafiltration to purify protein solutions, a dialysis buffer in the permeate is employed to set the pH in the protein solution. Failure to achieve the target pH may cause undesired precipitation of the valuable product. However, the pH in the permeate differs from that in the retentate, which contains the charged proteins. [1] Experimental optimization of the process conditions is time-consuming and expensive, while accurate theoretical predictions still pose a major challenge. Current models of dialysis account for the Donnan equilibrium, acid–base properties, and ion–protein interactions, but they neglect the patchy distribution of ionizable groups on the proteins and its impact on the solution properties. Here, we present a simple computational model of a colloidal particle with weakly acidic sites on the surface, organized in patches. [2] This minimalistic model allows systematic variation of the relevant parameters, while simultaneously demonstrating the essential physics governing the acid–base equilibria in protein solutions. Using molecular simulations in the Grand-Reaction ensemble, we demonstrate that interactions between ionizable sites significantly affect the nanoparticle charge and thereby contribute to pH difference between the permeate and retentate. We show that the significance of this contribution increases if the ionizable sites are located on a smaller patch. Protein solutions are governed by the same physics as our simple model. In this context, our results show that models which aim to quantitatively predict the pH in protein solutions during dialysis need to account for the patchy distribution of ionizable sites on the protein surface.

Keywords: colloidal nanoparticles, patchy distribution, Donnan effect, protein clustering/aggregation, pH.

References:

[1] Briskot T., Hillebrandt N., Kluters S., Wang G., Studts J., Hahn T., Huuk T., Hubbuch J. Modelling the Gibbs–Donnan effect during ultrafiltration and diafiltration processes using the Poisson–Boltzmann theory in combination with a basic Stern model. J. Membr. Sci, (648)2022, 120333.

[2] Pineda S.P., Blanco P.M., Staňo R., and Košovan P. Patchy charge distribution affects the pH in protein solutions during dialysis. Langmuir. 10.1021/acs.langmuir.4c0494.

Harnessing Coulombic Forces to guide Colloidal Self-assembly

Stefano Sacanna (New York University)

We present *polymer-attenuated Coulombic self-assembly*, a versatile strategy that uses neutral polymers to precisely tune the overlap of electrical double layers, enabling oppositely charged colloids in water to form a range of binary crystal structures selected by size ratio and stabilized for manipulation outside the solvent. Using an index-matched, fluorescent colloidal platform, we directly image crystallization in three dimensions with single-particle resolution, identify structures via simulated scattering, and track defect motion, melting, and twinning in real time. These experiments reveal a non-classical pathway in which amorphous precursors evolve into binary nanocrystals that grow by monomer addition, cluster capture, and oriented attachment. Continuous dialysis allows us to modulate interaction strength during growth, yielding diverse morphologies, including previously unreported hollow and composite heteroepitaxial crystals. This combination of tunable assembly and direct visualization offers a powerful model system for testing and refining theories of charged soft matter.

Counterion condensation, effective charge and ligand binding on macromolecules studied by PFG NMR

Ulrich Scheler (Leibniz Institute of Polymer Research Dresden)

The conformation and the stiffness of polyelectrolyte are determined by the repelling electrostatic force along the molecule that can be influenced by the ionic strength. The effective charge is reduced by the condensation of counterions if the charge density along the chain is so high that the thermal energy of the counterions is insufficient to escape it.

Pulsed-field-gradient (PFG) NMR measures the translation of molecules in solution distinguishing diffusion and directed flow. Both the self-diffusion coefficient and the electrophoretic mobility are measured on the same time and length scales. From the combination of both the effective charge of macromolecules is calculated and compared to the nominal charge permitting quantification of the counterion condensation. Charged small molecules may bind as ligands to macromolecules. Knowing the diffusion coefficient for both macromolecule and the free ligand compared to the effective diffusion coefficient in the interacting state the bound fraction and thus the dissociation constant is directly determined. Electrophoretic NMR allows determining the effective charge of both the macromolecule and the ligand and gives insight on the electrostatic interaction as a major contribution to binding. While the charge of a strong polyelectrolyte like PSS is independent of pH it varies for ligands like Lysine. This offers a possibility to investigate the strength of the interaction as a function of pH and thus the charge of the ligand. While the dominating interaction is the electrostatic interaction in this case there is a non-electrostatic component. Non-binding is found only when both the macromolecule and the ligand have a net charge of the same sign and the electrostatic effect repels them.

Using simulations to understand the role of charge interactions in drug delivery systems

Friederike Schmid (Johannes Gutenberg University Mainz)

Authors: Friederike Schmid, Jiajia Zhou, Jonas Lehnen, David Noel Zimmer, Giovanni Settanni

Electrostatic interactions play a central role in RNA/DNA delivery, yet their molecular-level consequences remain difficult to probe experimentally. Here, we use molecular simulations to explor how charge interactions shape the assembly and performance of two major classes of delivery vehicles: Polyplexes and lipid nanoparticles.

For polyplexes, where charge-charge interactions drive self-assembly, we simulate complexes formed by a single DNA molecule and block ionomers containing cationic and neutral hydrophilic blocks. The results show that ionomer sequence strongly affects polyplex compactness and microstructure, offering a possible explanation for experimentally observed differences in transfection efficiency [1]. We further find that the overall charge ratio between polyelectrolytes and RNA/DNA is the dominant factor determining polyplex composition. Near the isoelectric point, polyplexes form large aggregates, whereas away from it, smaller assemblies and even single-RNA complexes become accessible [2]. These trends are consistent with experimental observations in systems such as polyethylenimine with self-amplifying RNA.

In lipid nanoparticles, electrostatics govern both RNA binding and drug release. Our simulations reveal that the effective interactions between ionizable lipids and RNA switch from attractive to repulsive with pH [3], providing a potential trigger for release. Furthermore, we identify by which mechanisms electrostatic lipid–lipid interactions can promote lipid phase transitions that facilitate RNA escape [4].

Together, these findings highlight how charge interactions influence structure, stability, and release in RNA/DNA delivery systems.

References:

[1] The influence of block ionomer microstructure on polyplex properties: Can simulations help to understand differences in transfection efficiency? P. Heller, B. Weber, J. Zhou, D. Hobernik, M. Bros, F. Schmid, M. Barz, Small 13, 1603694 (2017). doi:10.1002/smll.201603694

[2] Assembly of polyplexes for RNA delivery J. Lehnen, J.M. Herrero, H. Haas, F. Schmid, G. Settanni, ChemRxiv preprint (2025). doi: 10.26434/chemrxiv-2025-k40pn

[3] pH-Dependent Behavior of Ionizable Cationic Lipids in mRNA-Carrying Lipoplexes Investigated by Molecular Dynamics Simulation G. Settanni, W. Brill, H. Haas, F. Schmid, Macrom. Rapid Comm. 43, 2100683 (2022). Doi: 10.1002/marc.202100683

[4] Transient interactions between cationic ionizable lipids and anionic lipids foster lamellar to hexagonal phase transition D.N. Zimmer, F. Schmid, G. Settanni, ChemRxiv preprint (2025). doi: 10.26434/chemrxiv-2025-rwb

Biomechanical resilience in centrosome kinetics

Marketa Schmidt Cernohorska (Jan Evangelista Purkyně University in Ústí nad Labem)

Centrosomes are essential protein organelles that orchestrate somatic cell division, enduring immense mechanical tension and forces as they organize the spindle and separate chromosomes. This constant stress necessitates unique **biophysical properties** and remarkable **intrinsic material resilience** within these soft matter structures. However, the exact nature of these properties and their maintenance mechanisms remain unknown, primarily due to the centrosome's minuscule size and complex, layered architecture of **disordered scaffolding proteins**. Existing microscopy techniques struggle to link their intricate structure with their mechanical behavior. My research aims to bridge this critical gap, advancing our understanding of fundamental assembly and mechanical principles, which is crucial for comprehending centrosome **pathology, particularly in early cancer development**. Uncovering centrosome biophysics extends beyond mere ultrastructural details; it delves into the interactions of scaffolding components. What truly gives centrosomes their unique **biomaterial properties**? Is it specific bonding between structural fibrillar components, or how they anchor microtubules? Unlike microtubules, built from globular tubulin, centrosomal scaffolds are mainly **fibrillar, intrinsically disordered proteins**. In this project, I study human centrosomes using an interdisciplinary approach: advanced microscopy to reveal coarse structure and material properties, molecular modeling to predict key proteins, and subsequent purification and condensation of these proteins into functional microtubule nucleation centers to test which combinations define centrosome mechanical integrity. This strategy connects local mechanics with global structural integrity, ultimately unveiling the molecular basis of centrosome function through its unique biophysical characteristics.

Monte Carlo Simulations of pH-sensitive polyelectrolyte microgels

Stefanie Schneider (RWTH Aachen University)

For weak polyelectrolytes (PE) as well as for weak polyampholytes (PA), not only the pH-pKA value but also the local electrostatic environment of the ionisable group determines the degree of ionisation and structural properties of the polymer. The proximity of already ionised groups, which is enforced by the interconnectivity of the polymer chain, influences the probability of additional groups to become ionised. Therefore, the degree of ionisation for polymers with different architectures differs from the ideal value, obtained for monomers at low concentrations. Linear PAs have been investigated theoretical [1] and in computer simulations [2]. PA with a network topology are interesting, because of their possible applications for the pH-triggered uptake and release of guest molecules.

Polyelectrolyte and polyampholyte microgels of different topologies have been investigated using constant pH-Monte Carlo simulations. Ionisation, swelling as well as the uptake and release of guest molecules were studied. [1-5]

References:

[1] C. Hofzumahaus, P. Hebbeker, S. Schneider, *Soft Matter*, **2018**, 14, 4087.
[2] C. Hofzumahaus, C. Strauch, S. Schneider, *Soft Matter*, **2021**, 17, 6029.
[3] C. Strauch, S. Schneider, *Soft Matter*, **2023**, 19, 938.
[4] C. Strauch, S. Schneider, *Soft Matter*, **2024**, 20, 1263.
[5] C. Strauch, L. Roß, S. Schneider, *Soft Matter*, **2024**, 20, 9664.

Exploring charge effects in soft matter: responsive particles, shape anisotropy and the role of charge patches

Peter Schurtenberger (Lund University)

Charges play a vital role for the stability of colloidal suspensions, their local and mesoscopic structure and dynamics and allow us to control and drive colloidal self-assembly. While charge effects are well characterised and understood for spherical hard colloids, the situation is less clear for more complex systems such as soft responsive particles like ionic microgels or strongly anisotropic particles with heterogeneous charge distribution like monoclonal antibodies.

Typical thermoresponsive ionic microgels possess a complex radial mass and charge density profile and often also carry long dangling chains. I will demonstrate how this complex particle architecture strongly influences the swelling behaviour of individual particles and the potential of mean force and thus the structural and dynamic properties of dilute and concentrated systems. I will also show how the interplay between the responsive nature of the particles and the large number of charges and counterions present allows us to induce and control self-assembly, e.g. the formation of colloidal molecules or binary crystals and the investigation of phase transitions, through variations of temperature and ionic strength and the application of external fields.

For anisotropic biological particles such as monoclonal antibodies [mAbs] charge effects are even more complex. Here the anisotropic Y-shaped structure combined with a complex and heterogeneous charge distribution requires much more refined models in order to describe the potential of mean force and the resulting structural and dynamic properties. These charges not only strongly influence solution properties, the colloidal stability and the phase behavior of the mAbs and thus their ability to be formulated into high concentration solutions required for pharmaceutical applications. They also need to be taken into account during the preparation of high concentration samples through ultrafiltration using centrifugal concentrators. Here the Gibbs-Donnan effect results in a concentration-dependant pH and ionic strength that in turn changes the charge state and the electrostatic contributions to the protein-protein interactions.

Charge in Double-Network Hydrogels: A Key to Understanding Toughening Synergy?

Tomáš Sedlačík (University of Chemistry and Technology, Prague)

The development of tough hydrogels with high strength and resilience has become a major scientific interest in recent years. As conventional hydrogels based on single networks (SN) are usually very soft or (if stiff then) brittle, tough hydrogels can largely expand the application potential of these materials.

Among several strategies, the creation of double networks (DNs) has proven particularly effective for achieving high toughness in hydrogels. DN hydrogels typically consist of a rigid first network, often based on a highly swelling polyelectrolyte, which serves as a sacrificial structure to dissipate mechanical energy applied to the hydrogel. Surprisingly, the influence of the charge density on the mechanical performance of DN hydrogels remained unexplored.

In our contribution to the field, we synthesized a range of double-network hydrogels from charged and neutral acrylic monomers, which exhibited varying combinations of strength, deformability, and mechanical reversibility. Based on these observations, we suggested that the mechanical performance of DN hydrogels can be controlled by the charge density of the first network independently of its (covalent) crosslinking density.

We took steps to validate this hypothesis by designing poly(2-oxazoline)-based hydrogels in which the charge density was precisely controlled using a thiol-ene "click" reaction. This approach yielded tough hydrogels with nearly complete mechanical reversibility.

Our findings suggest that this strategy for DN hydrogel design is broadly applicable to other systems, opening new pathways for the development of tough hydrogels with tunable mechanical properties. Furthermore, we believe our results could contribute to a deeper understanding of hydrogel toughening mechanisms.

Selective ion binding and uptake shape the microenvironment of biomolecular condensates

Iris Smokers (Radboud University)

Biomolecular condensates modulate various ion-dependent cellular processes and can regulate subcellular ion distributions by selective uptake of ions. To understand these processes it is essential to uncover the molecular grammar governing condensate-ion interactions. In this work, we use NMR spectroscopy of ions and model condensate components to quantify and spatially resolve selective ion binding to condensates and find that these interactions follow the "law of matching water affinities", resulting in strong binding between proteins and chaotropic anions, and between nucleic acids and kosmotropic cations. Ion uptake into condensates directly follows binding affinities, resulting in selective uptake of strong-binding ions, but exclusion of weak-binding ions. Ion binding further shapes the condensate microenvironment by altering the composition, viscosity and interface potential. Such changes can have profound effects on biochemical processes taking place inside condensates, as we observe for RNA and DNA duplex formation. These findings provide a new perspective on the role of condensate-ion interactions in cellular bio- and electrochemistry and may aid design of condensate-targeting therapeutics.

Charged for attraction: How biomolecular condensates pull chromosomes together

Valerio Sorichetti (Institute of Science and Technology Austria)

The coacervation of charged polymers is an important driver for the formation of biomolecular condensates. Recent experiments suggest that this mechanism also controls the clustering of eukaryotic chromosomes during the late stages of cell division [1,2]. In this process, inter-chromosome attraction is driven by the condensation of cytoplasmic RNA and Ki-67, a charged intrinsically disordered protein that coats the chromosomes as a brush. Attraction between chromosomes has been shown to be specifically promoted by a localized charged patch on Ki-67, although the physical mechanism remains unclear [2]. To elucidate this process, we combine coarse-grained simulations and analytical theory to study the RNA-mediated interaction between charged polymer brushes on the chromosome surfaces [3]. We find that the charged patch on Ki-67 leads to inter-chromosome attraction via RNA bridging between the two brushes, whereby the RNA preferentially interacts with the charged patches, leading to stable, long-range forces. By contrast, if the brush is uniformly charged, bridging is basically absent due to complete adsorption of RNA onto the brush. Moreover, the RNA dynamics becomes caged in presence of the charged patch, while remaining diffusive when the charge is uniform. Our findings suggest that cells could control the forces exerted by biomolecular condensates by adjusting the way charges are distributed on proteins, providing a potential strategy for regulating biological organization.

References:

[1] S. Cuylen-Haering, M. Petrovic, A. Hernandez-Armendariz, M. W. Schneider, M. Samwer, C. Blaukopf, L. J. Holt, and D. W. Gerlich, *Nature* **587**, 285 (2020)

[2] A. Hernandez-Armendariz, V. Sorichetti, Y. Hayashi, Z. Koskova, A. Brunner, J. Ellenberg, A. Šarić, and S. Cuylen-Haering, *Molecular Cell* **84**, 3254 (2024).

[3] V. Sorichetti, P. Robin, I. Palaia, A. Hernandez-Armendariz, S. Cuylen-Haering, A. Šarić, *Charge distribution of coating brush drives inter-chromosome attraction*, biorXiv 2024.12.01.626236.

Diverse non-equilibrium behavior of protein condensates in electric fields

Jennifer Tersteegen (Aalto University)

Jennifer Tersteegen, Antti Mäkynen, Adam Harmat, Maria Sammalkorpi, Markus B. Linder, Jaakko V. I. Timonen

Liquid-liquid phase separation (LLPS) of biomolecules is key to biological processes and biomaterial formation (1). Since living systems operate under non-equilibrium conditions, factors like concentration and pH shifts impact LLPS. Understanding this dynamic behavior is essential to grasp cellular functions and biomaterial assembly.

Here, we study experimentally an engineered spider silk protein in vitro that undergoes LLPS and investigate its non-equilibrium behavior under the influence of an external electric field. The studied multidomain protein features an intrinsically disordered middle block, flanked by globular terminal domains. Brightfield microscopy and digital holographic microscopy reveal diverse, voltage-dependent behavior, including condensate movement, interfacial changes, reversible dissolution of condensates, and electro-convective patterns. We associate this behavior with electric field-driven pH changes due to electrolysis of water as well as electrophoresis and electrodiffusiophoresis. The pH changes affect, e.g., the charges of protein terminal domains – our previous work indicates that the interaction of the terminal domains is essential for the studied protein's ability to undergo LLPS (2). Understanding the far-from-equilibrium behavior of protein condensates can facilitate actively driven and controlled materials assembly.

References: (1) Mohammadi, P.; Aranko, A. S.; Lemetti, L.; Cenev, Z.; Zhou, Q.; Virtanen, S.; Landowski, C. P.; Penttilä, M.; Fischer, W. J.; Wagermaier, W.; Linder, M. B. *Commun Biol* **2018**, 1 (1), 86.

(2) Fedorov, D.; Roas-Escalona, N.; Tolmachev, D.; Harmat, A. L.; Scacchi, A.; Sammalkorpi, M.; Aranko, A. S.; Linder, M. B. *Small* **2024**, 20 (13), 2306817.

Unifying the dynamics of viscoelastic liquids across the complex coacervation phase diagram: time-polyelectrolyte-salt superposition

Mehdi Vahdati (Institute Charles Sadron)

The dynamics and structure were investigated for polyelectrolyte-rich liquids across the high-salt region of the complex coacervation phase diagram of high molecular weight poly(sodium 4-styrenesulfonate), PSS, and poly(diallyldimethylammonium chloride), PDADMAC. The total concentration of polyelectrolytes was increased at different added KBr concentrations ([KBr]) to obtain liquid complex coacervates (CC) and single-phase, high-salt polyelectrolyte solutions. The dynamic response of these entangled polymer liquids was found to be self-similar at each [KBr], allowing a time-polyelectrolyte superposition using only a polyelectrolyte concentration-dependent horizontal shift factor. This self-similarity was further found among all the samples at different [KBr], allowing the construction of a universal master curve unifying the dynamics of all the samples by applying a second, salt-dependent horizontal shift factor. The complex coacervate dynamics were found to have a very strong dependence on the experimentally determined PEs concentration, while salty solutions of non-interacting PEs behaved as polymers in good solvent. The extreme scaling in the case of the CC defies the predictions for entangled associating polymers, probably due the very high polymer concentration and the large number of stickers per chain. Despite the absence of effective stickers in the salty solutions of fully doped polyelectrolytes, they can mimic the viscoelastic response of the CCs up to the solubility limit of the PEs. We called these materials quasi-complex coacervates (quasi-CCs) to distinguish them from both CC and single-polyelectrolyte solutions. Small angle X-ray scattering (SAXS) revealed that PSS/PDADMAC CC, their quasi-CCs, and a PSS solution at the same total polymer and salt concentration have different nanostructures. Unifying the dynamics of viscoelastic liquids across the high-salt region of the phase diagram, time-polyelectrolyte-salt superposition may be regarded as a route to predict the composition and properties of these polyelectrolytes-rich materials.

Harnessing the Triboelectric Effect for Patchy Particles Synthesis: Properties and Self-Assembly

Peter D J van Oostrum (University of Natural Resources and Life Sciences, Vienna)

Inverse patchy colloids (IPCs) are nano-to-microscale particles characterized by distinct oppositely charged regions, or ”patches,” on their surfaces [1]. This inhomogeneous charge distribution leads to orientation-dependent attractive and repulsive interactions between particles, giving rise to rich self-assembly patterns influenced by external parameters like pH and salt concentration [2]. Here, we introduce a novel and simple method for synthesizing silica-based IPCs with two positively charged patches based on the triboelectric effect. To facilitate the visualization of patches via confocal and scanning electron microscopy, the positive patches were labeled with fluorescent dyes and gold nanoparticles respectively. To prevent particles from entering the van der Waals attraction region and minimize steric interactions, the IPCs were also coated with the neutral polymer, Pluronic F-127. This coating promotes colloidal stability while maintaining the selective attraction between the patchy and non-patchy regions via overlapping electric double layers. We investigated the self-assembly behavior of IPCs in function of the pH which tunes the relative charges at a fixed salt concentration [3]. Our method provides a simple yet versatile approach for synthesizing IPCs for studies in colloidal science and materials engineering.

References:

[1] Virk et al, J. Phys.: Condens. Matter 35 174003 (2023)
[2] E. Bianchi et al, Current Opinion in Colloid & Interface Science, 30, 18 (2017)
[3] Virk et al, in preparation

On Complex(ed) Relations: the Power and Peculiarities of Nanoscopic Polyelectrolyte-based Particles

Ilja Voets (Eindhoven University of Technology)

Polyelectrolyte complexation is a powerful approach to generate dynamic materials with adaptive properties and precision polymer and hybrid protein-polymer nanoparticles, which can be tailored to meet requirements specific to their application in e.g. nanomedicine. In this lecture I will discuss the preparation, properties, and (dis)assembly pathways of hydrocolloids comprising at least two oppositely charged (bio)macromolecules. Particularly appealing of such particles is their modulatory: morphology, size, stability, and function are tunable. Systematic studies of structure-property relations allow tailoring of some of these features as desired. Rational design remains however one of the grand challenges, especially for those systems and conditions where kinetic traps are prominent. I will highlight recent work on complex coacervate core micelles, single-enzyme nanoparticles, and polyelectrolyte complexation out-of-equilibrium, that is, orchestrated by clock reactions and induced by polymerization. The impact of polymer architecture on C3Ms as well as novel routes to generate complex coacervate-based particles with high stability and a tunable lifetime will be discussed. Finally, the opportunities of polymerization-induced electrostatic self-assembly (PIESA) to prepare customized hydrocolloids will be addressed. This technology has recently been introduced as an attractive means to prepare polyelectrolyte complex particles on large scale under mild conditions. Extraordinary morphologies have been reported, but these are often unstable. We recently discovered a novel strategy to regulate the polymerization. I will address how this switchable, electrostatically templated polymerization offers excellent control over the assembly pathway to custom-tailor the hydrocolloids that form and gain more in-depth insight in the PIESA process.

Phase Separation of DNA: From Fundamentals to Artificial Cells

Andreas Walther (Johannes Gutenberg University Mainz)

Building on our recent discovery of temperature induced phase separation of single-stranded DNA, I will highlight in this talk aspects of sequence specificity, the use of the phenomenon to build artificial cells, as well as discuss a new type of non-Fickian diffusion and how to install a metabolism for information processing.

Posters

Thermal properties of a knotted diblock copolymer ring

Neda Abbasi (University of Szczecin)

The phase transitions and geometrical characteristics of diblock copolymers have been studied extensively, however, relatively few studies have focused on knotted structures under varying the monomer distributions and changing the solvent quality with temperature. In this study, we present an extensive computational study to investigate how topological constraints and the block lengths affect the behaviour of a single diblock copolymer ring. We used the Wang-Landau Monte Carlo algorithm and a coarse-grained modelling on a simple cubic lattice in an implicit solvent to explore the thermal and structural properties of such systems. We employed the AB model where there are self-repulsive interactions between A type monomers, self-attractive interactions between B type monomers and interactions between A and B types monomers are neutral. In this model, the solvent is considered good for A type and bad for B type monomers at low temperature. Key properties, such as the heat capacity, the radius of gyration for individual blocks and the entire diblock ring, the number of contacts between monomers of the same and different types (AA, BB, and AB), as well as the distance between the centers of mass of the two blocks have been computed. Our simulations show two order phase transitions corresponding to mixing-unmixing of the A and B monomers and the melting of the compact state formed at low temperatures by the B monomer. Our results show that by a suitable choice of topology, it is possible to tune the phase transition temperature at which the rearrangement of the system occurs. Furthermore, we used the HP protein-folding model for the diblock copolymer to make a comparison with the AB model. We have determined the extent to which the repulsive interactions between type A monomers influences the physical properties of the system.

Coarse-graining of slit-confined star polymers in solvents of varying quality

Reyhaneh Afghani Farimani (University of Vienna)

We investigate star polymers with varying functionalities and under varying solvent conditions confined within a slit geometry. Our approach involves an accurate estimation and validation of the effective interaction by directly computing the force between a pair of star polymers and comparing the radial distribution function from monomer-resolved molecular dynamics simulations with that obtained through Monte Carlo simulations using the effective interaction. Our findings reveal significant sensitivity in the radial distribution function to subtle variations in the tail of the interaction potential, particularly in dilute regimes. Furthermore, we employ a morphological model to analyze the interpenetration of the star polymers, demonstrating that reducing the functionality leads to a marked increase in the interpenetration of these polymeric systems. We establish that solvent quality has minimal impact on the degree of interpenetration whereas the star functionality affects it markedly, leading to enhanced faceting and reduced interpenetration for as the number of arms grows. These results are particularly relevant for enhancing our understanding of polymeric materials' rheological and mechanical properties.

Ion-Specific Effects on the Conformation of DNA oligo-Catenanes

Chara Alexiou (University of Vienna)

The scope of the work presented here is the computational investigation of the effects of counterion valency on the ensuing effective interactions between topologically interlinked DNA ring molecules. Atomistic molecular dynamics (MD) simulations were performed for double stranded DNA [2]-catenanes in low to moderate ionic strength solutions of monovalent sodium and divalent counterions calcium and magnesium solutions. Prominent effects of the ion type on the separation of the center-of-masses of the individual minicircles, as well as their preferred relative orientations have been established. An interesting interplay arises upon increasing ionic strength of divalent counterions, depending on the contour length of the individual DNA minicircle constituents: short

DNA minicircles give rise to a non-monotonic behavior that comprises sequential elongation and contraction regimes of the catenane, but longer minicircles give rise only to contracted catenane conformations.

Charge Regulation in G2 PAMAM–Peptide Conjugates for Gene Delivery

Pablo M. Blanco (Norwegian University of Science and Technology)

Poly(amidoamine) (PAMAM) dendrimers are promising vectors for gene delivery due to their high cationic charge, which enables strong DNA binding, protection from nucleases, and facilitation of cellular uptake. Additionally, their ability to buffer endosomal acidification may promote endosomal escape via osmotic swelling and rupture. While high-generation PAMAM dendrimers efficiently condense nucleic acids, their high charge density is associated with significant cytotoxicity. In contrast, lower-generation dendrimers, such as G2, are less toxic but show limited nucleic acid condensation. To address this trade-off, we explore G2 PAMAM dendrimers conjugated with peptide tails of varying sequences. This design aims to retain DNA-binding capability while reducing cytotoxicity. We employed a combination of coarse-grained constant-pH simulations, potentiometric titrations, and DNA precipitation assays to evaluate their gene delivery potential. First, our coarse-grained models were benchmarked against experimental titration data, showing a very good agreement. We then used simulations to measure the potential of mean force between DNA and different PAMAM–peptide conjugates at different pH values and analyzed the charge regulation resulting from their interaction. Complementary, we performed DNA precipitation assays at different pH and concentration of the PAMAM-peptide conjugates. Our integrated computational and experimental approach provides a mechanistic understanding of charge regulation in PAMAM–peptide conjugates and paves the way for rational design of low-generation dendrimer-based vectors with tunable charge properties and reduced cytotoxicity.

Non-Fickian diffusion in aggregates of a polyampholytic disordered protein β-casein

Saikat Chakraborty (Grenoble Alpes University)

β-casein is a polyampholytic intrinsically disordered protein (IDP) with block-copolymer-like decoration of charged residues. Most of its charges are concentrated in hydrophilic N-teminal, and the C-terminal is highly hydrophobic. In aqueous solutions, the IDP is known to form micelles. For all measured concentrations of such samples beyond the critical micelle concentration, a non-Fickian wave-vector dependence of the spectral broadening is observed in incoherent quasi-elastic neutron scattering. The profiles are similar to those for globular proteins in crowded environment. To seek the origin of such anomaly, we employ atomistic molecular dynamics simulations of the IDP in explicit water. Through simulation generated spectra of single and multiple chains, we show that aggregation prompts the non-Fickian behavior. We reveal that at the core of the aggreagate residues experience a self-induced crowding and exhibit low mobility. Whereas, closer to the surface of the aggregate, the chains move faster. With an analytical model, we establish such dynamic heterogeneity as the microscopic origin of the anomalous diffusion.

A model for predicting polyelectrolyte self-assembly in solution: effects of pH, salt concentration, and mixing ratio

Gabriel Federico Debais (Aalto University)

I am applying to participate in the workshop on Charged Soft Matter: Bridging Theory and Experiment to present my recent theoretical advances in the modeling of charged polymers, specifically polyelectrolyte self-assembly in solution. My research focuses on studying physical principles behind diverse polyelectrolyte assemblies soft matter systems. I have developed a mean-field level theory that provides a unified framework for describing polyelectrolyte complexation in solution and the layer-by-layer (LbL) self-assembly [1]. The model incorporates chemical equilibrium concepts to capture ion pairing and counterion release, accurately predicting phase diagrams and the impact of pH and salt concentration on film growth [1]. We connect the findings with the "universal curve" linking experimental coacervation and LbL assembly proposed by Larson et al. [2]. Here, I demonstrate how my modelling approach captures further pH, salt concentration, and mixing ratio influence the assembly behavior of charged polymer systems, in agreement with key experimental observations, including pH-dependent shifts in coacervation and the variation of critical salt concentrations [1,3]. The findings set the model as a predictive tool for understanding polyelectrolyte assembly phase behavior across a wide range of systems. My system is fully composed of charged macromolecules in polar solvent (water), accompanied by salt ions, and I am pursuing an interdisciplinary experiments-and-simulations driven advance to understanding these, right at the core of the workshop.

References:

[1] G. Debais and M. Tagliazucchi, Macromolecules 55(12), 2022.

[2] A. Salehi, P.S. Desai, J. Li, C.A. Steele, R.G. Larson, Macromolecules 48(2), 2015.

[3] C.I. Eneh, K. Nixon, S. Lalwani, M. Sammalkorpi, P. Batys, J. Lutkenhaus, Macromolecules 57(5), 2024.

Molecular architecture modulates self-assembly and micellar rheology of model ionic surfactant systems

Steph Flores (University of Manchester)

Understanding the rheology of micellar systems is critical for advancing soft matter physics and enabling innovations in consumer product formulations. In micellar systems comprising ionic surfactants, predictive models are uniquely challenging to construct due to the combined effects of salt screening and surfactant polydispersity on micelle self-assembly. In this work, we demonstrate how the amphiphilic nature of ionic surfactants governs self-assembly and rheological properties by systematically varying surfactant geometry in model systems of sodium lauryl ether sulfates. Key structural features – hydrophilic headgroup size (degree of ethoxylation), hydrocarbon tail length, and solution polydispersity – are controlled to uncover three distinct regimes in viscosity and the salt concentration at the peak of salt curves. In systems containing multiple headgroup types, peak viscosity trends are found to depend on the average ethoxy linker number, while the salt concentration required to achieve peak viscosity correlates with compositional balance. The observed Gaussian symmetry in viscosity trends underscores the intricate relationship between molecular structure and macroscopic behaviour in these systems. Our results contribute to the development of predictive models that bridge molecular-scale surfactant behavior with bulk rheological phenomena, offering pathways for improved formulations and advancements in the physics of self-assembled systems.

Inferring Microstructural Characteristics from the Yielding Behavior of Jammed Carbopol Suspensions

Francesca Galluzzi (Foundation for Research and Technology-Hellas)

In recent years, significant progress has been made in understanding the dynamics of jammed soft colloidal particles, which are prevalent in both natural and industrial applications. To gain deeper insight into yield stress, it is crucial to establish a link between macroscopic mechanical response and local microstructure.

Carbopol, a widely used industrial material, serves as a prime example, yet its microstructure remains largely unresolved. To address this, we have developed a method that leverages the rheological response of structurally well-characterized soft materials in the jamming regime. By identifying characteristic rheological patterns, we correlate their behavior with internal microstructural properties.

Our analysis distinguishes three types of jammed materials: emulsions with constant particle volume, microgels undergoing osmotic compression (deswelling), and star polymers that compress and interpenetrate. This classification is based on transient shear stress studies and flow curve analysis, providing a valuable framework for linking microstructural features to jamming and yielding behavior.

By analyzing the rheological data of Carbopol, we can determine whether its particles generally deform at a constant volume, deswell, and/or interpenetrate, indicating the presence of dangling ends; due to this information we can conclude the microstructure of this industrial material.

Computational inverse homogenization approach for predicting the mechanical properties of randomly distributed ellipsoidal inclusions of composite materials

Panagiotis Ilia (The Cyprus Institute)

Designing the next generation of circular materials requires a comprehensive understanding of their mechanical performance. Here, we present a computational framework for the in-silico design and optimization of AgReCOMPOSITES-sustainable, circular materials derived from recycled plastic and biochar produced from agricultural and livestock waste. This framework combines hierarchical homogenization and Finite Element Methods with experimental data to predict the mechanical performance of biochar-polymer composites, enabling the optimization of mixing ratios and geometrical configurations for superior functionality. A key focus is on the random distribution of the ellipsoidal nanoparticle reinforcements—which significantly influences the mechanical response of the composite material. In this work we developed an inverse numerical homogenization model that predicts the inclusions properties with excellent agreement to experimental data. We extend these methodologies to AgReCOMPOSITES, showcasing the potential and challenges of the computational inverse homogenization methodology in transforming sustainable, circular materials design.

Modeling acid-base properties of copolypeptides of glutamate and lysine with tyrosine

Vojtěch Keprta (Charles University)

Polypeptides are an essential part of biological systems. If they contain amino acids with acidic or basic side chains, they can carry a charge due to dissociation reactions depending on the pH. Polypeptides can thus be considered weak polyelectrolytes, and describing their pH-responsive behavior is important for understanding their biological functioning as well as for potential applications. Molecular simulations in particular have a long history in this regard. In this work, a coarse-grained computer model of two different polypeptides is created and it is investigated how parameters of the model such as the level of detail in it or system parameters such as chain length and salt concentration affect the behavior of these polypeptides. A significant difference is observed between the ionization degree at varying pH values of polypeptides modeled with our two different coarse-grained models (”one-bead” and ”two-bead”) owing to the differing effective distances between charged residues in each of them. The observed effects of chain length and ionic strength on the ionization behaviour of the polypeptides is in line with previous work on weak polyelectrolytes for both of our models. Further experimental work has been carried out in our group to allow for a comparison with these results and a potential validation of our modelling.

Advancing Drug Vehicle Applications by Nanocarrier Capabilities Enhancement

Miroslava Nedyalkova (University Fribourg)

Molecular dynamics and SAXS simulations were used to study micelle formation with SDS, imidazole-, and pyrimidine-based ionic liquids (ILs) encapsulating drugs of varying polarity: estradiol, ibuprofen, and caffeine. The computational protocol enabled atomic-level insights into self-assembly, drug localization, and aggregation behavior over time. SAXS-derived form factors and scattering patterns revealed denser, more stable IL micelles – especially with pyrimidine ILs – versus SDS. Drug encapsulation depth varied by polarity. These results, consistent with SAXS-based phase diagrams, underscore the advantage of simulations in predicting micelle structure and optimizing drug delivery design, offering a powerful tool for guiding experimental formulations and accelerating the development of next-generation therapeutic carriers.

pH-Responsive Charge Regulation in polypeptides

Ipsita Padhee (Charles University)

Understanding the behaviour of weak polyelectrolytes, like polypeptides, as a function of pH is crucial for biological and material applications, as the charge regulation affects structure, stability and function. Therefore, we investigated the charge regulation of a polypeptide sequence of Glutamate and Tyrosine (EEEEY), focusing on its degree of ionization as a function of pH. Computationally, coarse-grain modelling was used while experimentally, potentiometric titration and fluorimetry were used to calculate the degree of ionization and pKa values and compared with the Henderson-Hasselbalch (HH) equation.

The comparison between the experimental and simulation result shows that the simple models can predict the real ionization behaviour of peptides by following a similar overall trend. Whereas some deviations from the simple model arise due to the complex electrostatic interactions. Qualitatively, these computational approaches are reliable in support of peptide charge regulation and ionization dynamics, but improvements in modelling are needed for quantitative accuracy.

Active colloids at fluid-fluid interface

Amir Sheikh Shoaei (Dresden University of Technology)

Active particles can use energy from their environment to achieve directed motion. Depending on the characteristics of each particle and the confining environment, different phenomena can arise at both the single-particle and collective levels. Of special interest are fluid-liquid interfaces, where microorganisms such as bacteria and algae accumulate and form biofilms. These interfaces often have curved, non-flat shapes, such as water droplets, that impose unique constraints on the motion of active particles. To better understand the emerging behaviors, here we experimentally show the behavior of bottom-heavy Janus particles on curved droplets. We study the influence of bottom-heaviness on the dynamics of individual particle movement and the resulting collective behavior. Janus particles exhibit gravitaxis due to their displaced center of gravity relative to their hydrodynamic center. Furthermore, we show that motility-induced phase separation occurs as a result of the nonhomogeneous density distribution of particles at the interface. Our results aim to provide experimental understanding for the recent theoretical studies on the dynamics of active particles at fluid-fluid interfaces and modified motility-induced phase separation due to the curvature of the interface. Moreover, this study provides insight into the behavior of biological matter moving near non-flat surfaces.

Dialysis of polyelectrolyte solution

Eliška Stančíková (Charles University)

My work focuses on the dialysis of polyelectrolyte solutions, with an emphasis on quantifying the Donnan effect by measuring pH differences (ΔpH) across a semipermeable membrane. The motivation stems from the observed discrepancy between ΔpH in dialyzed protein solutions and predictions based on the Donnan theory, which lacks accuracy in conditions relevant to manufacturing of pharmaceutical proteins. The primary research question is whether experimental ΔpH values can be more accurately captured by molecular simulations using coarse-grained (CG) model of PMAA, incorporating electrostatic interactions. Using poly(methacrylic acid) (PMAA) as a model system, we developed a dialysis protocol for systematic pH measurements and performed potentiometric titrations to observe ionization behavior at different PMAA concentrations. Our hypothesis was that the Donnan model overestimates ΔpH, while simulations including interactions should better reflect experimental data. The results confirmed significant ΔpH values due to the Donnan effect, particularly at high polymer concentration and low ionic strength. The Donnan theory overestimated ΔpH in these regimes, but CG simulations accounting for interactions showed improved, though not perfect, agreement with experiment – especially when ΔpH was derived from Cl^- ion distributions. These findings suggest that including interactions in theoretical models is essential to accurately capture non-ideal behavior in polyelectrolyte systems, particularly under conditions where the Donnan effect is most pronounced.

Entangled and Charged: The Subtle Interplay of Topology and Electrostatics in Charged Polymers

Andrea Tagliabue (University of Genoa)

Topological constraints such as knots and links play a central role in determining the structural, dynamical, and rheological properties of polymeric and soft matter systems.[1] These features are not only fundamental in synthetic metamaterials, but are also widespread in biological systems – including both linear and circular DNA[2], proteins[3] with knotted or slipknot topologies, and highly catenated mitochondrial DNA networks such as those found in kinetoplasts[4] – where they influence organization, function, and dynamics across multiple scales. Notably, many of these biological systems are charged. In this contribution, I will explore the complex interplay between topological constraints (knots and links) and electrostatic interactions in charged polymers, a coupling that often gives rise to unexpected nonmonotonicities and nontrivial trends. I will highlight how the conformational, thermodynamic, and dynamical behavior of these systems can be finely tuned by modifying both the chemical properties of the chains (e.g., the distribution of charges along the backbone[5, 6]) and environmental conditions such as pH[7], ionic strength[8], and the nature of counterions[8, 9]. Mastering this tunability holds promise for the creation of novel stimuli-responsive metamaterials and for advancing our understanding of the physiological behavior of topologically complex biomacromolecules.

Refereces:

[1] Tubiana et al., Physics Reports 2024 1075, 1-137

[2] Micheletti, DNA Knots. In: Tezuka, Y., Deguchi, T. (eds) Topological Polymer Chemistry. 2022 Springer

[3] Faísca, Computational and Structural Biotechnology Journal 2015, 13, 459-468

[4] Michieletto, Nucleic Acids Research 2025, 53, 2

[5] Tagliabue et al., ACS Macro Lett. 2021, 10, 11, 1365–1370

[6] Chiarantoni et al., Macromolecules 2025, 10.1021/acs.macromol.5c00099

[7] Tagliabue et al., J. Phys. Chem. B 2020, 124, 14, 2930–2937

[8] Tagliabue et al., Macromolecules 2022, 55, 23, 10761–10772

[9] Tagliabue et al., J. Phys. Chem. B 2024, 128, 17, 4183–4194

Polymer–Surface Interactions in Ceramic Formulations: A Molecular Simulation Study of PMA and PAA on Amorphous Silica

Andrea Tagliabue (University of Genoa)

The ceramic industry is expanding across multiple sectors, but rising energy costs, mainly from thermal treatments (drying and sintering), threaten its competitiveness. Reducing water in formulations, without losing suitable rheological properties, is a key strategy to lower energy demand[1]. To this end, we investigate, both computationally and experimentally, the possible usage of superplasticizer additives, specifically polycarboxylate ethers (PCEs), already widely used in water-based materials like cement[2]. In this contribution, we present the first step of our simulation effort: the study of the interaction between polymethylacrylate (PMA) and polyacrylate (PAA)—which form the backbone of PCEs—and amorphous silica, a major constituent of typical ceramic formulations. Using atomistic molecular dynamics simulations and enhanced sampling protocols, we systematically explore the influence of polymer tacticity, surface ionization, and solution ionic strength on polymer–surface interactions. Our simulations reveal that, despite polymers and surface being like-charged, their attraction increases with surface ionization. This effect becomes particularly pronounced in the presence of $CaCl_2$, where divalent counterions dramatically enhance the polymer–surface affinity.

Refereces:
[1] Mezquita et al., How to reduce energy and water consumption in the preparation of raw materials for ceramic tile manufacturing: Dry versus wet route, Journal of Cleaner Production, 168, 2017,1566-1570
[2] Lei et al., 40 years of PCE superplasticizers - History, current state-of-the-art and an outlook, Cement and Concrete Research, 157, 2022, 106826

Contact Forces in Microgel Suspensions

Fran Ivan Vrban (University of Ljubljana)

Several classes of colloidal materials are based on deformable particles, a notable example being microgel sols. The interactions among such microscopic constituents upon contact are rather complex, and they include elastic and dissipative terms. Despite many advances in the understanding of the elastic interactions, the many-body nature of these forces is hardly ever considered and the model which is best-known and typically used is still the Hertzian interaction. Here we theoretically explore the so-called liquid drop model of deformable particles. To provide a coarse-grained description of the contact interaction in the partial, advanced, and complete faceting regimes, we employ three distinct geometrical approximations for the deformed particle shape, involving truncated spheres, superballs and spheropolyhedral shapes, respectively. We compare the deformation energy obtained using these three approximations to the exact numerical results for selected local configurations and we determine the range of indentations where the drop-drop interaction is pairwise additive, which is generally quite limited, mostly to small deformations. Our work provides an insight into the and a basis for a consistent description of the mechanics, elasticity, and phase behavior of suspensions of microgels and nanocolloidal particles.

Phase separation in elastic polymer networks

Takahiro Yokoyama (Leibniz Institute of Polymer Research Dresden)

Phase separation in polymer networks, from synthetic gels to biopolymer networks, significantly influences their structural and mechanical properties. While previous studies suggest that network mechanics regulate phase separation of the network itself and the embedded (complex) liquid, the fundamental principles governing this interaction remain poorly understood. To address this knowledge gap, we used molecular dynamics (MD) simulations to investigate the elasticity and phase separation behavior of polymer networks with varying characteristic length scales. Specifically, we systematically varied the chain contour length, persistence length, and entanglement length. Our simulations identified two distinct phase separation behaviors depending on the network state: macrophase separation, and microphase separation characterized by finite-sized domains. We found that the key factors to achieve microphase separation are local chain bending rigidity and topological constraints, quantified by persistence length and entanglement length. These intrinsic length scales play crucial roles in regulating both the elastic properties and phase separation behavior in elastic polymer networks.