Coarse-graining the finer structure of macromolecular interactions

Ljubljana, August 27–30, 2023

About the symposium

The symposium "Coarse-graining the finer structure of macromolecular interactions," will take place in the vibrant city of Ljubljana, Slovenia, from August 27 to 30, 2023. This event aims to gather distinguished researchers, both experimentalists and theorists, from across the globe to delve into the most exciting prospects and challenges in the field. The main objective of the symposium is to foster an environment of intellectual exchange and collaboration, where the participants can share their insights and discoveries concerning macromolecular interactions. The symposium will feature a series of 30-minute talks, which will serve as the backbone of the event. Alongside the scheduled talks, plenty of time will be left for participants to engage in in-depth conversations, allowing for the exploration of ideas, novel approaches, and potential collaborations. Apart from the scientific program, attendees can enjoy the charming atmosphere of Ljubljana. The city's mix of history and modernity provides a perfect environment for networking and socializing.

Organizing Committee

Matej Kanduč (chair), Jožef Stefan Institute, Ljubljana, Slovenia
Anže Božič, Jožef Stefan Institute, Ljubljana, Slovenia
Matej Praprotnik, National Institute of Chemistry and Faculty of Mathematics and Physics, University of Ljubljana, Ljubljana, Slovenia
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KEMIJSKI INŠTITUT

PROGRAM

Monday, August 28		
09:00	Matej Kanduč	Opening remarks
09:15	David Andelman	One Hundred Years of Modeling Electrolytes: What's New with the Theories of Debye and Onsager?
09:45	Vincent Démery	Pair Correlation in Out of Equilibrium Mixtures
10:30	*coffee break*	
11:00	*(chair: X. Man)* Christian Holm	Simulating Acid-Base Equilibria in Polymeric Systems
11:30	Jalal Sarabadani	Polymer Translocation in an Environment of Active Rods
12:00	Daniel Harries	Determination of Thermodynamic Parameters in Molecular Simulations: Insights into Lipid Nanodiscs and Sugar Glass
12:30	*lunch break*	
14:00	*(chair: G. Pabst)* Achille Giacometti	On the Effects of Chirality and Charge on the Stability of Liquid Crystal Phases
14:30	Ali Naji	Highly Tunable Casimir Interactions Mediated by Ferrofluids
15:00	Horacio V. Guzman	RNA Adsorption onto Flat and Membranous Substrates from Multiscale Models
15:30	*coffee break*	
16:00	*(chair: A. Naji)* Şahin Büyükdağlı	Self-Consistent Analysis of Electrostatic Correlation Effects in Bulk and Nano-Confined Liquids with Composite Structure
16:30	Yevgeniy Mamasakhlisov	The Polyelectrolyte with a Disorder Over Short-Range Interactions
Tuesday, August 29		
09:00	*(chair: M. Praprotnik)* Kurt Kremer	Playing with Entanglements to Structure Polymer Materials
09:30	Cristian Micheletti	Designed Self-Assembly of Molecular Knots, Links and Topological Gels
10:00	Xingkun Man	Onsager Variational Theory of Gel Swelling
10:30	*coffee break*	
11:00	*(chair: L. Tubiana)* Roya Zandi	Virus Symmetry-Breaking, Elasticity and Self-Assembly
11:30	Nataša Adžić	All-DNA Constructs in a Construction of Unconventional State of Matter
12:00	Jure Dobnikar	Self-Assembly of Viral Capsids and Packing of Genome
12:30	*lunch break*	

14:00	*(chair: A. Šiber)* Georg Pabst	Why Can Asymmetric Lipid Bilayers Be so Much More Rigid than Equally Composed Symmetric Ones?
14:30	Saša Svetina	On Curvature Dependent Interaction between Membrane Channels and Lipid Bilayer
15:00	Gregor Cevc	Molecular Structure, Interactions, and Boundary Conditions Effects on Polar Lipids Aggregates in Water, as Macromolecular Assemblies Model
15:30	*coffee break*	
16:00	*(chair: J. Dobnikar)* David Dean	Single File Diffusion in Spatially Inhomogeneous Systems
16:30	Roland Netz	Projection Methods for Non-Markovian Non-Equilibrium Systems
19:30	*conference dinner at the Manna restaurant*	
Wednesday, August 30		
09:00	*(chair: A. Giacometti)* Tomer Markovich	Odd Viscosity in Chiral Active Matter: Coarse Graining of the Kinetic Energy is not Unique
09:30	Ignacio Pagonabarraga	Hydrodynamically-Induced Emergent Structures in Active and Driven Matter
10:00	Yael Avni	The Non-Reciprocal Ising Model
10:30	*coffee break*	
11:00	*(chair: M. Krajnc)* Antonio Šiber	Extreme Mechanics of Pollen Deformation
11:30	Siniša Pajević	Delay Plasticity: Complex Systems with Adaptive Time Delays
12:00	Hugues Chaté	Extreme Deformability of Active Crystals
12:30	*lunch break*	
14:00	*(chair: C. Micheletti)* Silvia Tomić	From Solid State to Soft Matter Physics: Structural Dynamics of DNA Explored by Dielectric and Infrared Spectroscopy
14:30	Luca Tubiana	From Kinetoplast DNA to Bio-Inspired Topological Supramolecular Materials and Back
15:00	Artem Badasyan	Spin Model of Water and Post-Processing of Protein Folding Experiments

TABLE OF CONTENTS

ALL-DNA CONSTRUCTS IN A CONSTRUCTION OF UNCONVENTIONAL STATE OF MATTER

Nataša Adžić
Institute of Physics, Belgrade, Serbia

All-DNA constructs are macromolecules that are solely composed of short segments of DNA chains joined together to form dendrimeric structures [1]. We first take a look at equilibrium properties of a single molecule of various dendrimer generations immersed in an ionic solution at room temperature. The results extracted from simulation and experiment show how the given macromolecules exhibit a behavior atypical for other dendrimer families, classifying all-DNA constructs as good candidates for nanocariers [2]. Then we delimit our study on the second generation of all-DNA constructs only and we investigate self-assembly of these molecules in dense solutions. Both theoretic and experimental results demonstrate that the system stays in a liquid phase characterized by an anomalous structure factor behavior. Last, we modify the structure of all-DNA constructs of the first and the second generation by inserting a polymer chain as a connector between two all-DNA building blocks. We show that self-assembly of these molecules leads to the formation of soft cluster crystals, periodic structures with multiple site occupancy [3].

[1] Y. Li, Y. Tseng, and D. Luo, Nat. Mater. **3**, 38 (2004).
[2] C. Jochum, N. Adžić, E. Stiakakis, T. L. Derrien, D. Luo, G. Kahl, and C. N. Likos, Nanoscale **11**, 1604 (2019).
[3] E. Stiakakis, N. Jung, N. Adžić, T. Balandin, E. Kentzinger, U. Rucker, R. Biehl, J. Dhont, U. Jonas, and C. N. Likos, Nat. Commun. **12**, 7167 (2021).

ONE HUNDRED YEARS OF MODELING ELECTROLYTES: WHAT'S NEW WITH THE THEORIES OF DEBYE AND ONSAGER?

D. Andelman[1], Y. Avni[1,2], R. M. Adar[3], H. Orland[4], and R. Podgornik[5]

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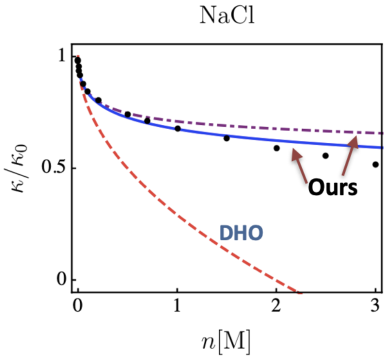
The Poisson-Boltzmann theory stems from the pioneering works of Debye and Onsager and is considered even today as the benchmark of ionic solutions and electrified interfaces. It has been instrumental during the last century in predicting charge distributions and interactions between charged surfaces, membranes, electrodes, macromolecules, and colloids. After a brief review of the Poisson-Boltzmann theory, I will review the seminal work of *Onsager-Samaras* for the surface tension of electrolytes and will present a field theoretical approach [1] that improves on the original result by taking into account ionic-specific effects and relating our result to the Hofmeister series. I will then discuss the conductivity of ionic solutions, which is arguably their most important trait, being widely used in electrochemical, biochemical, and environmental applications. The *Debye-Hückel-Onsager* theory successfully predicts conductivity at very low ionic concentrations of up to a few millimolar, but there is no well-established theory applicable at higher concentrations. I will present our conductivity study [2,3] using a stochastic density functional theory, paired with a modified Coulomb interaction that accounts for the hard-core repulsion between the ions. The modified potential suppresses unphysical, short-range electrostatic interactions, which are present in the *Debye-Hückel-Onsager* theory. Our analytical and compact results show very good agreement with experimental data for conductivity up to 3 molars, without any fit parameters.



[1] T. Markovich, D. Andelman, and R. Podgornik, Langmuir **33**, 34 (2017).
[2] Y. Avni, R. M. Adar, D. Andelman, and H. Orland, Phys. Rev. Lett. **128**, 098002 (2022).
[3] Y. Avni, D. Andelman, and H. Orland, J. Chem. Phys. **157**, 154502 (2022).

THE NON-RECIPROCAL ISING MODEL

Y. Avni[1], M. Fruchart[2], D. Martin[3,4], D. Seara[1], and V. Vitelli[1,3]

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Newton's third law – the reciprocity of interactions between two particles – translates the conservation of momentum at the molecular scale. Out of equilibrium, complex macromolecules can violate this symmetry. Examples include activator-inhibitor dynamics and auto-catalytic chemical reactions, where one molecular species enhances the abundance of another species, yet the latter diminishes the abundance of the former, leading to *non-reciprocal* effective interactions. Coarse-graining the dynamics of such systems within the mean-field approximation suggests that they can undergo phase transitions to time-dependent phases in which the order parameter oscillates. We study the fate of such phase transitions in spatially extended noisy systems using a non-reciprocal generalization of the Ising model. Our results show that globally synchronized oscillations are unstable in two dimensions due to the formation of spiral defects but they are stabilized in three dimensions. We also identify two oscillatory regimes in 3D: noisy-homogeneous oscillations and droplet-induced oscillations. In the latter regime, global synchronization decreases with increased local synchronization. Finally, we argue that any amount of non-reciprocity prevents the existence of static ordered phases.

SPIN MODEL OF WATER AND POST-PROCESSING OF PROTEIN FOLDING EXPERIMENTS

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Materials Research Laboratory, University of Nova Gorica, Nova Gorica, Slovenia

The presence of several distinct minima in nearest-neighbor potentials in polymers makes it possible to describe polymer conformations in terms of discrete isomeric states, naturally leading to spin language. Using this general approach, a decade ago we have suggested the Hamiltonian formulation for the Zimm and Bragg model of protein conformations [1,2]. Later we have augmented the model by an oversimplified spin model for water, resulting in both cold and hot denaturations [3]. We construct the Statistical Mechanics for the model and get access to its Thermodynamics. Resulting order parameter and specific heat expressions are successfully fit to available experimental data [4]. Thanks to solid and traceable theoretical foundations, the procedure provides better quality fits as compared to the state-of-the-art two-state model, routinely used to process protein folding experiments.

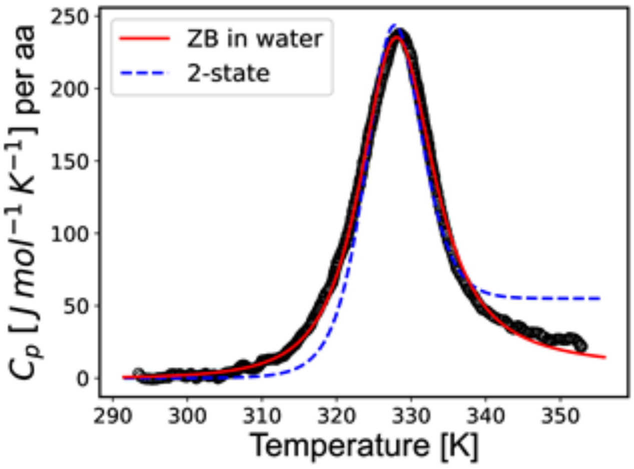

Fig. 1. DSC experimental data points (dots) for S44[A] mutant of T4 lysozyme [5] fitted to 2-state (dashed blue) and to ZB model in water (red solid).

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[3] A. Badasyan S. A. Tonoyan, A. Giacometti, R. Podgornik, V. A. Parsegian, Y. S. Mamasakhlisov, and V. F. Morozov, Phys. Rev. E. **89**, 022723 (2014).
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[5] J. H. Carra., E. C. Murphy, and P. L. Privalov, Biophys. J. **71**, 1994 (1996).

CHARGE-REGULATED ONSAGER-DUPUIS THEORY

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The original Onsager-Dupuis theory is a phenomenological approach to the electrostatic properties of ice. It generalizes linearized Poisson-Boltzmann theory by an additional structural polarization potential caused by the defect structure of ice. Recently, within a field-theoretic derivation of a generalized Poisson-Boltzmann theory for ‘structured’ liquids [1], we have recovered Onsager-Dupuis theory as a lowest-order approximation to water structure in liquid electrolytes. Following the recent derivation of the general boundary conditions for structured liquids [2], we present results from an application of our theory to the case of charge-regulated surfaces.

[1] R. Blossey and R. Podgornik, Phys. Rev. Res. **4**, 023033 (2023).
[2] R. Blossey and R. Podgornik, J. Phys. A: Math. Theor. **56**, 025002 (2023).

SELF-CONSISTENT ANALYSIS OF ELECTROSTATIC CORRELATION EFFECTS IN BULK AND NANO-CONFINED LIQUIDS WITH COMPOSITE STRUCTURE

S. Büyükdağlı

Department of Physics, Bilkent University, Ankara, Turkey

The composite structure of the electrolyte solutions involved in biological processes requires the characterization of the underlying many-body interactions within theoretical frameworks able to account for the distinct interaction strengths of the separate liquid components. In this talk, I will discuss statistical mechanical formulations of charged liquids capable of treating asymmetrically the solvent background, and the mono- and multivalent ion components of the electrolyte according to their individual electrostatic coupling strength and concentration.

The first part of the talk will be devoted to correlation effects in *implicit solvent* electrolyte mixtures confined to nanopores. Via the weak-coupling (WC) variational-level inclusion of the monovalent salt component and the virial treatment of the multivalent ions, I will derive from the electrostatic Schwinger-Dyson (SD) identities a set of self-consistent (SC) equations incorporating the weak- and strong-coupling interactions of the different charge species on an equal footing [1]. This framework will be shown to provide a SC route to the previously developed dressed-ion theory of mixed electrolyte solutions [2,3].

By coupling this electrostatic formalism with hydrodynamic equations, I will obtain a unified theory of charge and polymer transport through confined nanopores. Within this correlation-corrected transport theory, I will investigate the electrohydrodynamic mechanism responsible for the emergence of the experimentally observed negative streaming currents in anionic nanochannels [4,5]. Then, the transport formalism will be applied to carbon-coated nanopores characterized by the giant membrane permittivity condition [6]. In the corresponding electrostatic configuration, the theory predicts a novel molecular transport mechanism enabling the dielectric control of the polymer translocation speed and direction via the simple adjustment of the electrolyte composition. Finally, if time permits, I will discuss the salt-induced suppression of the dielectric response in bulk electrolytes. I will show that the solution of the *solvent-explicit* SD equations via the WC treatment of the solvent background and the virial treatment of the ion component allows to capture accurately the experimentally observed linear decay of the dielectic permittivity with added dilute salt [7].

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[4] S. Büyükdağlı, J. Phys. Chem. B **124**, 11299 (2020).
[5] F. H. J. van der Heyden, D. Stein, and C. Dekker, Phys. Rev. Lett. **95**, 116104 (2005).
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MOLECULAR STRUCTURE, INTERACTIONS, AND BOUNDARY CONDITIONS EFFECTS ON POLAR LIPIDS AGGREGATES IN WATER, AS MACROMOLECULAR ASSEMBLIES MODEL

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[†]Deceased

Solvated (typically hydrated) polar lipids form various aggregates. Their properties are telling for other macromolecular self-assemblies, too, being all sensitive to molecular' structure and boundary conditions as co-determinants of the decisive forces. The main, van der Waals, attractive force can be modelled in detail [1]. The consensus about the fluctuations and hydration caused repulsion (and in case attraction) modelling is still elusive, however. This includes the question of interplay between fluctuations, their intra-and interfacial correlations, and hydration force [2].

To improve experimental data basis for future modelling of molecular assemblies we studied un/binding of different polar lipid vesicles to a lipid monolayer at an air-water interface using surface selective techniques (ellipsometry, X-rays reflectivity). The independent variables were system temperature, the chemical composition (carbons number per aliphatic chain {12-18}, phospholipid headgroups methylation {phospho-ethanolamine-N-methyl$_n$, $0 \le n \le 3$, i.e., -ethanolamine (PE)} to -choline (PC)} in the monolayer and in the similar or dissimilar vesicles, as well as the average size and lamellarity of the latter; the main observables were surface coverage (vesicles adsorption) and the adsorbed aggregates transformation (vesicles deformation). This confirmed an increase of attraction and a decrease of molecular exchange-rate between monolayer and vesicles with aliphatic chains prolongation. Temperature (through molecular packing density) and especially phospholipid headgroups have more diverse and instructive effects. PC vesicles adsorb extensively to a PE monolayer if their aliphatic chains are ordered, and far less otherwise. Their binding to a PC monolayer is 50% less extensive, at most, and requires molecular 'fluidity' in vesicles and order in the monolayer plus interfacial 'softness' (i.e., the $P'_{\text{ß}}$ phase) to occur. Mono- or dimethylation of amino-groups decreases/increases adsorption of vesicles with fluid/ordered chains to a gel phase PC monolayer, by affecting interfacial polarity and lipid headgroups propensity for H-bonding, and thus water binding, as well as molecular ordering and correlations. Any realistic model of interactions between (macro)molecular assemblies, and their consequences, should therefore also allow for interfacial softness and intra- or interfacial correlations.

[1] R. Podgornik, G. Cevc, and B. Žekš, J. Chem. Phys. **87**, 5957(1987).
[2] J. G. Hedley, H. Berthoumieux, and A. A. Kornyshev. J. Phys. Chem. C **127**, 8429 (2023).

CHARGE REGULATION EFFECTS IN NANOPARTICLE AND POLYELECTROLYTE PHASE BEHAVIOR

T. Curk

Johns Hopkins University, Baltimore, USA

Polyelectrolytes, hydrogels and nanoparticles in solution acquire charge through the dissociation or association of ionic surface groups. Thus, a proper description of their electrostatic interactions requires the use of *charge-regulating* boundary conditions rather than the commonly employed constant-charge approximation. Using a Monte Carlo/molecular dynamics scheme that dynamically adjusts the charges of individual ionizable groups we investigate nanoparticle self-assembly and calculate the pH–temperature phase diagrams of linear polyelectrolytes as well as hydrogels. Using histogram reweighting techniques, we show how the charge regulation effects lead to discontinuous coil–globule and collapse–swelling transitions. The extent of the discontinuous region and the existence of two critical points at low and high pH values depends sensitively on the size of the counterions. Computational results are supported by an analytical mean-field theory. These insights are used to design efficient hydrogel-based nano-actuators, and moreover, provide a possible explanation on why it is difficult to electrostatically self-assemble nanoparticle and colloidal crystals.

SINGLE FILE DIFFUSION IN SPATIALLY INHOMOGENEOUS SYSTEMS

D. S. Dean

Laboratoire d'Ondes et Matière d'Aquitaine, University of Bordeaux, Bordeaux, France

We study the effect of spatially-varying potential and diffusivity on the dispersion of a tracer particle in single-file diffusion. Non-interacting particles in such a system exhibit normal diffusion at late times, which is characterised by an effective diffusion constant D_{eff}. Here we demonstrate the physically appealing result that the dispersion of single-file tracers in this system has the same long-time behavior as that for Brownian particles in a spatially-homogeneous system with constant diffusivity D_{eff}. Our results are based on a late-time analysis of the Fokker-Planck equation, motivated by the mathematical theory of homogenization. The findings are confirmed by numerical simulations for both annealed and quenched initial conditions.

PAIR CORRELATION IN OUT OF EQUILIBRIUM MIXTURES

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G. Palumbo[5], D. Dumont[6] and P. Damman[5]

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Mixtures can be put out of equilibrium by different means: with a differential external forcing, by putting the species in contact with different thermostats, or by introducing non-reciprocity in the interactions. In the two last cases, which can be mapped onto each other, pair correlations remain isotropic but display also specific non-equilibrium features. I will discuss how they arise at the three-body level using different formalisms valid for weak interactions or low density.

SELF-ASSEMBLY OF VIRAL CAPSIDS AND PACKING OF GENOME

J. Dobnikar[1], J. D. Farrell[1], T. Curk[3], and R. Podgornik[2]

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[2] University of Chinese Academy of Sciences, Beijing, China
[3] Johns Hopkins University, Baltimore, USA

Assembly of viral capsids containing genetic material, is a key process in viral reproduction cycle. The capsid assembly differs qualitatively among viruses: bacteriophages and double stranded DNA viruses initially assemble empty capsids, into which DNA is driven by an ATP packaging motor; the single stranded RNA/DNA viruses package their genomes concurrently with the capsid assembly, resulting in a co-assembly of the virus genome and capsid proteins. We have explored a simplified model of an elastic filament confined to a sphere with replica-exchange MD simulations combined with energy minimization approaches. In contrast to a general assumption that viral DNA is packed in an inverse spool configuration, we show that compartmentalization into multiple domains (either multiple spools or intertwined rings resembling twisted topological links) is a preferred ground state at high densities. We further explored the role of the kinetics of packing via nonequilibrium simulations of DNA pushed into a capsid by a molecular motor. We observe structures with spool-like symmetry in the outer shells and melted or twisted-nematic core regions, which are in agreements with recent experimental observations. Finally, we studied the co-assembly process with ssRNA and capsid proteins with icosahedral symmetry. We explored the stability of assembled virions and found that it depends in a complex fashion on both genome topology (branchedness) and degree of confinement. Our model predicts that MS2 bacteriophage should prefer a linear genome topology, which is compatible with the Hamiltonian path hypothesis of RNA conformation in the virions.

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ANOMALOUS UNDERSCREENING IN ELECTROLYTES

C. E. Woodward[1] and J. Forsman[2]

[1]PEMS, University of New South Wales, Canberra, Australia
[2]Theoretical Chemistry, Lund University, Lund, Sweden

This presentation includes a summary of some interesting and conflicting (?) results established by many different groups in this field, from experimental as well as theoretical investigations. We will also discuss our recent efforts, where we import simulation data to classical density functional theory (DFT) to arrive at limiting electrostatic decay lengths, which generally deviate from the standard Debye screening length. We then adopt this combined simulation/DFT approach to restricted primitive model (RPM) electrolytes, with an emphasis on parameters for which recent simulations by Härtel et al. [Phys. Rev. Lett. **130**, 108202 (2023)] have established underscreening behaviour. We corroborate that RPM electrolytes with a rather long Bjerrum length can display substantial underscreening, and we find nice agreements between the Decay lengths obtained from the long-range structure tails, and predictions by our DFT. In a concentrated "aqueous" RPM, on the other hand, our DFT predicts a rather strong overscreening., and simulations verify that correlations in this case are dominated by excluded volume (packing), with no significant long-ranged tail. We end by discussing clustering effects, and some remaining discrepancies between experiments and theoretical results obtained with the RPM.

ON THE EFFECTS OF CHIRALITY AND CHARGE ON THE STABILITY OF LIQUID CRYSTAL PHASES

A. Giacometti

Università Ca' Foscari, Venice, Italy
ECLT European Centre for Living Technology, Venice, Italy

In this talk, I will describe recent efforts by our group on the stability of some special liquid crystal phases along two lines. First, I will discuss the effect of chirality on the self-assembly and phase behavior of rigid helices whose surface is partially attractive and partially repulsive, and illustrate the connection between microscopic chirality of the molecules and chirality of the phase [1-3].

In the second part, I will discuss the stabilization of liquid crystalline phases by electrostatic interactions, and its application to the correct interpretation of phase transitions of rod-like virus particles at very low ionic strength [3-4].

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[2] L. Dal Compare, F. Romano, J.. Wood, and A. Widmer-Cooper, and A. Giacometti, under review (2023).
[3] J. Wood, T. Hudson, A. Giacometti, and A. Widmer-Cooper, under review (2023).
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[5] L. Dal Compare, E. Grelet, and A. Giacometti, in preparation (2023).

DETERMINATION OF THERMODYNAMIC PARAMETERS IN MOLECULAR SIMULATIONS: INSIGHTS INTO LIPID NANODISCS AND SUGAR GLASS

D. Harries

Institute of Chemistry and the Fritz Haber center, The Hebrew University, Jerusalem, Israel

Extraction of thermodynamically instructive parameters from molecular dynamics simulations poses a continuous challenge. In this presentation, I will introduce methodologies that we have developed, which enable the accurate determination of two important parameters: the bending elastic constant of lipid mesophases and the free energy associated with the hydrogen bond in solutions [1-3]. To illustrate the practical implementation of these methodologies, I will showcase their application in two distinct systems: lipid nanodiscs and the glassy state of aqueous sugar mixtures.

[1] G. I. Olgenblum, L. Sapir, and D. Harries, J. Chem. Theor. Comp. **16**, 1249 (2020).
[2] L. Sapir and D. Harries, J. Chem. Theor. Comp. **13**, 2851 (2017).
[3] I. Schachter, C. Allolio, G. Khelashvili, and D. Harries, J. Phys. Chem. B **33**, 7166 (2020).

SIMULATING ACID-BASE EQUILIBRIA IN POLYMERIC SYSTEMS

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[2]Department of Physical and Macromolecular Chemistry, Charles University, Prague, Czech Republic

In this talk I will review our progress of the recent years for the study of macromolecular weak polyelectrolyte systems. In the first part I will shortly review several algorithms for studying such systems [1-3], followed by a presentation of selected applications to various macromolecular systems [4-6].

[1] J. Landsgesell, C. Holm, and J. Smiatek, Eur. Phys. J. Special Topics **226**, 725 (2017).
[2] J. Landsgesell, P Hebbeker, O Rud, R Lunkad, P Košovan, and C Holm, Macromolecules **53**, 3007 (2020).
[3] J. Landsgesell, D. Sean, P. Kreissl, K. Szuttor, C. Holm, Physical Review Letters 122, 208002 (2019).
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PLAYING WITH ENTANGLEMENTS TO STRUCTURE POLYMER MATERIALS

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Entanglements are known to dominate the rheological properties of long chain polymer melts and dense solutions. Their properties and consequences lead to the generally accepted and well established reptation/tube model, which is at the basis of our understanding of many properties and processes. However, beyond analysing their effects and understanding the very nature of entanglements, one also can take the approach to use them to manipulate and structure materials. The talk will give a few such examples ranging from melts of non-entangled to very long, highly entangled polymer systems. By appropriately mapping chemical chain lengths onto idealized bead spring models one can (semi-) quantitatively compare simulation and experiment and predict new materials. Based on predictions from simulations we recently prepared stable nanoporous polymer films just by mechanical deformation. Furthermore, we applied a new data driven approach to determine the glass transition temperature of polymer melts and (ultra) thin films.

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VAN DER WAALS INTERACTION BETWEEN THERMALLY UNDULATING LIPID BILAYERS

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Starting from a microscopic model of a lipid bilayer which accounts consistently for both the orientation and dipole fluctuations of the lipid molecules, we determine the van der Waals free energy between two thermally undulating lipid bilayers and its undulation fluctuation correction at leading perturbative order. We find that in the absence of undulations, the free energy is attractive and contains four terms, one of which varies as $(L + D)^{-4}$ another as $(L - D)^{-4}$ and two as L^{-4} (where L is the mean inter-bilayer separation and d is the bilayer thickness). The undulation correction enters at the same order and interpolates between two limiting values as the inter-bilayer distance is varied: firstly, the undulations strengthen the van der Waals attraction with increasing inter-bilayer distance, with the enhancement saturating in the far-field limit. Secondly, owing to the steric effect, the undulation-induced attractive enhancement decreases as the separation distance is reduced [1].

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THE POLYELECTROLYTE WITH A DISORDER OVER SHORT-RANGE INTERACTIONS

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We consider a generic flexible polyelectrolyte comprised of equally charged monomers with the disorder conditioned by the short-range features only like e.g. single-stranded RNA. Similar systems have been studied before in [1-4]. We have addressed the statistical mechanical model of a three-dimensional polymer chain with randomly quenched interactions. The pe charge per monomer is assumed, where e is the electron charge and $0 < p < 1$. The position of a monomer is considered in a continuous way as $r(t)$, where $t \in [0, N]$ and N is the dimensionless length of the chain. The random sequence of the chain assumes that the type of each monomer is described by independent random variable drawn with the same Gaussian probability law.

The free energy and the density profile of the system without salt are calculated in the general case. The numerical results are obtained for the system of two infinite plates separated by *2a* distance with the polyelectrolyte chain between. The effects of the disorder are analyzed. In particular, the enhancement of condensation is shown in comparison with disordered cases in the dense regions of the system (Fig. 1).

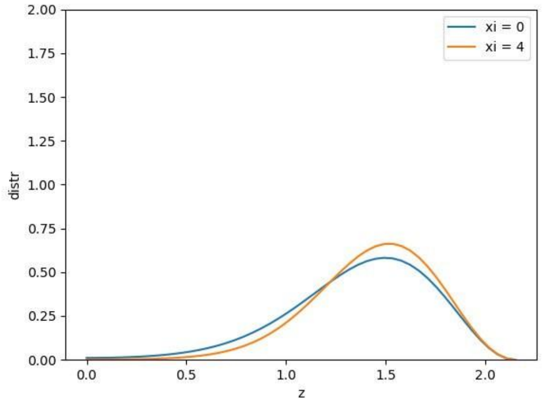

Fig. 1. The monomers density distribution vs. inter-plate half-distance for different values of disorder.

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ONSAGER VARIATIONAL THEORY OF GEL SWELLING

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Swelling of polymer gels is one of the classical problems in polymer science and technology. In the swelling process, the solvent diffusion is coupled with the deformation of the polymer network and is coupled with the stress field created in the gel. Such coupling is called diffusio-mechanical coupling. In recent years, we developed a diffusio-mechanical theory for gel swelling, which is based on the Onsager variational principle. In this talk, I will give three examples of using such a theory to study the swelling of gel, including (a) swelling dynamics of a disk-shaped gel [1], (b) bending of gel induced by liquid penetration [2] and (c) accelerating the bending of a gel using mechanical constraints [3]. Analytical expressions are given for the maximum curvature, the equilibrium curvature, and the characteristic time of gel swelling. This finding brings valuable approach in designing soft robotics and healthcare devices, and is subject to experimental test.

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ODD VISCOSITY IN CHIRAL ACTIVE MATTER: COARSE GRAINING OF THE KINETIC ENERGY IS NOT UNIQUE

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Chiral active materials are composed of complex molecules that break both parity and time reversal symmetry (TRS) at the microscale. This is generally a result of continuous injection of energy and angular momentum through local torques. Realizations of such fluids are found in a variety of systems across length scales, from nanoscale biomolecular motors, actomyosin networks, and microscale active colloids, to macroscale-driven chiral grains. An important consequence of the breaking of parity and TRS is the possible appearance of odd viscosity. Unlike regular viscosity that dissipates energy, odd viscosity is 'reactive' and can be obtained using a Hamiltonian theory with no need of adding dissipation. Importantly, Onsager reciprocal relations predict that such odd viscosity only appears when TRS is broken. In this talk I will introduce the concept of total momentum, which accounts for both the center-of-mass (CM) and angular momenta and show that in chiral active materials the distinction between this total momentum and the CM momentum is crucial. Specifically, I will discuss two potential coarse-grainings of the kinetic energy that results in very different dynamics: Both exhibit odd viscosity, but one of which obeys Onsager's relations, and one does not. Arguing that the latter gives the real dynamics brings about the conclusion that the mere existence of spin angular momentum density due to local torques leads to odd viscosity, but also breaks Onsager's reciprocity relations, which results in non-Hermitian dynamical matrix. When interactions are included phenomenologically, we find regions in in the parameter space in which novel 3D mechanical waves propagate in the bulk, and regions in which they are mechanically unstable. The lines separating these regions are continuous lines of exceptional points, suggesting of a non-reciprocal phase transition.

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DESIGNED SELF-ASSEMBLY OF MOLECULAR KNOTS, LINKS AND TOPOLOGICAL GELS

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Supramolecular constructs with complex topologies are of great interest across soft-matter physics, biology and chemistry, and hold much promise as metamaterials with unusual mechanical properties. A particularly challenging problem is how to rationally design, and subsequently realize, these structures and the precise interlockings of their multiple molecular strands. Here we report on the combined use of theory and simulations to obtain complex supramolecular constructs via programmed self-assembly. Specifically, by controlling the geometry of the self-assembled monomers we show that the assembly process can be directed towards "privileged", addressable topologies of molecular knots, and extended linked structures, such as Olympic gels and catenanes. We conclude presenting an overview of the unique static and dynamical properties of linear catenanes. The talk will cover results based on publications [1-4]

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For an actual hands-on demonstration of the designed self-assembly of "macroscopic" trefoil knots see the video at this link: www.youtube.com/watch?v=XKsuMlp2PLcA .

HIGHLY TUNABLE CASIMIR INTERACTIONS MEDIATED BY FERROFLUIDS

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Ferrofluids are stabilized suspensions of superparamagnetic (e.g., magnetite) nanoparticles in a nonmagnetic host liquid (e.g., kerosene or water) [1]. They have emerged as an important class of materials with tunable magnetic properties [2]. This has made ferrofluids relevant also in the context of Casimir interactions (see, e.g. [3,4]). This is because, in small-scale devices such as micro and nanoelectromechanical systems, the typically attractive Casimir force that acts between their miniaturized parts can produce undesirable effects such as stiction and system malfunction. Consequently, controlling the Casimir interaction has become an important area of study. To our knowledge, the Casimir interaction mediated by a ferrofluid layer confined between two solid substrates has so far been investigated only in the case of isotropic ferrofluids. Other effects such as size polydispersity of the constituent magnetic nanoparticles and/or their surface coating have also not been considered before. We study these latter factors and their impact on the Casimir pressure in a three-slab system consisting of dielectric (e.g., gold-SiO_2) substrates confining a thin ferrofluid film. We also extensively study the role of field-induced structural anisotropy when the system is subjected to an external magnetic field. In this case, the constituent nanoparticles can undergo reversible restructuring by self-assembling into higher-order structures (specifically linear magnetic chains). We show that the formation of even relatively short chains (comprising two to ten nanoparticles) in the ferrofluid can engender drastic modifications in the Casimir pressure acting on the substrates; hence, not only the sign of the Casimir pressure can conveniently be tuned but its magnitude can also be varied over a striking range of several decades as the field strength (or concurrently also the temperature or volume fraction of nanoparticles) is adjusted only over a modest range of realistic values. In particular, a longitudinally applied field (along the surface normal of the substrates) is found to facilitate a much greater degree of sign and magnitude tunability compared to a transverse field. The underlying mechanisms at work here are elucidated by an in-depth analysis of transverse magnetic and transverse electric modes within the Lifshitz formalism, illustrating how the specific axis of anisotropy due to the field-aligned chains in the ferrofluid can regulate the resulting Casimir pressure.

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PROJECTION METHODS FOR NON-MARKOVIAN NON-EQUILIBRIUM SYSTEMS

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Most physical systems are interacting many-body systems, one typically describes their kinetics in terms of low-dimensional reaction coordinates. The dynamics of such reaction coordinates is governed by the generalized Langevin equation (GLE), an integro-differential stochastic equation, and involves a memory function, which describes how the reaction coordinate dynamics depends on its previous values. The GLE is thus an intrinsically non-Markovian description of the dynamics of a system in terms of coarse-grained variables. We have recently introduced a novel hybrid projection scheme that allows to extract the GLE parameters from time series data in a form that is convenient for analytic and numerical treatments [1] and have shown that memory effects are significant for protein folding [2,3].

Non-equilibrium effects are characterized by slowly relaxing transient variables and can be described by a time-dependent Hamiltonians, in fact, non-equilibrium systems typically exhibit pronounced memory effects. Two systematic approaches for such systems will be discussed: Using an appropriate projection, a non-equilibrium formulation of the GLE is presented. As an alternative approach, data filtering is shown to lead to modified GLEs that are particularly useful for the treatment of time series data from non-physical sciences.

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WHY CAN ASYMMETRIC LIPID BILAYERS BE SO MUCH MORE RIGID THAN EQUALLY COMPOSED SYMMETRIC ONES?

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Native plasma membranes contain a large number of lipid species that distribute asymmetrically between the two leaflets of the bilayer. For example, mammalian plasma membranes are composed of an outer leaflet enriched in choline phospholipids, such as phosphatidylcholine and sphingomyelin, while phosphatidylserine and phosphatidylethanolamine are confined to the inner leaflet [1]. Searching for distinct physical behavior of asymmetric bilayers prompted us to determine the structure and bending rigidity of minimal plasma membrane mimics composed of diverse lipids [2, 3].

Most strikingly, we observed that asymmetric bilayers with inner leaflets composed of phosphatidylethanolamine/phosphatidylserine mixtures and outer leaflets enriched in phosphatidylcholine were much stiffer than equally composed but symmetric bilayers. Moreover, these asymmetric bilayers were also much stiffer than symmetric bilayers composed of their cognate leaflets. None of the existing theoretical frameworks [4] was able to explain this anomalous stiffening. We speculate that lipid-specific interactions (H-bonding, electrostatic interactions,…) may increase the weight of short-wavelength undulatory modes in membranes by inducing a coupling at distances smaller than the membrane thickness.

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HYDRODYNAMICALLY-INDUCED EMERGENT STRUCTURES IN ACTIVE AND DRIVEN MATTER

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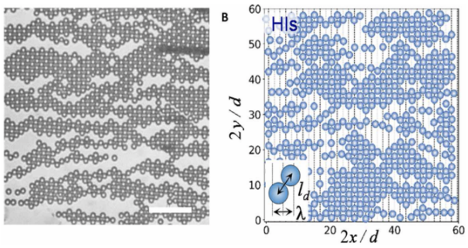
Suspensions intrinsically out of equilibrium disturb the liquid medium in which they are embedded as a result of nonequilibrium processes, such as chemical reactions, or inhomogeneous thermal heating. These are intrinsically out of equilibrium systems, which makes them very versatile, with a natural tendency to self-assemble. Due to their small size, these out of equilibrium dynamical states generate flows at low Reynolds numbers that induce long range hydrodynamic interactions. These interactions have profound effects in the transport, spontaneous self-assembly and emergence of stable mesoscopic structures.

In this talk I will address the role that hydrodynamics play in the rectification mechanism that leads to particle motion, as well as the possibility that hydrodynamic instabilities lead to novel, dynamically-stabilized mesostructures. I will discuss the impact that these mechanisms have in the emergence of patterns and different type of morphological structures in active suspensions. I will combine theoretical simple models and computer simulations to gain insight in the role of hydrodynamics in these out of equilibrium system.



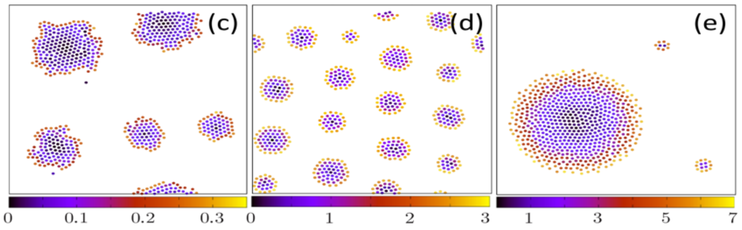


Figure 1: Anisotropic clusters of dipolar colloids popelled by a rotating magnetic field controlled by the hydrodynamic coupling.

Figure 2: Self assembled clusters of rotating colloids. Particles attract and interact hydrodynamically. The relative strength of the attraction with respect to hydrodynamic force controls the characteristic size of the self-organized discoidal clusters.

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DELAY PLASTICITY: COMPLEX SYSTEMS WITH ADAPTIVE TIME DELAYS

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It is increasingly evident that adaptive regulation of signal timing in neural systems is present and occurs during learning through a mechanism of myelin plasticity [1]. Myelination might not be the only mechanism by which neural systems adjust their timing. More importantly, other biological and complex systems might also require the use of adaptive time delays, or latencies, to control system stability, synchronizability, and other system-level properties. Here, we discuss the effects that interaction delays can have in complex systems, including complex networks of molecular interactions, and explore the advantages and consequences of delay plasticity – i.e., the ability of some complex systems to adaptively adjust their inherent interaction time delays. While it is difficult to envision that the latencies in molecular interactions themselves can be adaptive, their temporal characteristics can facilitate delay plasticity in neural systems [1].

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POLYMER TRANSLOCATION IN AN ENVIRONMENT OF ACTIVE RODS

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Using a combination of Langevin dynamics simulations and isoflux tension propagation (IFTP) theory the dynamics of a flexible linear polymer translocation through a nanopore into an environment composed of repulsive active rods is considered in two dimensions. It is demonstrated that the rod activity induces a crowding effect on the polymer, leading to a time-dependent effective net force that facilitates translocation into the active environment. Moreover, it is shown that the rods facilitate translocation to the *trans* side even when there are initially more monomers on the *cis* than on the *trans* side [1]. Structural analysis of the translocating polymer reveals that active rods induce a folded structure to the trans-side subchain in the case of successful translocation events. By keeping the initial number of monomers on the *cis*-side subchain fixed, a state diagram for successful events as a function of the rod number density is mapped out for a variety of system parameters. This reveals competition between facilitation by the rods at low densities and crowding that hinders translocation at higher densities [2].

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EXTREME DEFORMABILITY OF ACTIVE CRYSTALS

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We demonstrate that two-dimensional crystals made of active particles can experience extremely large spontaneous deformations without melting. Using particles mostly interacting via pairwise repulsive forces, we show that such active crystals maintain long-range bond order and algebraically-decaying positional order, but with a decay exponent whose value is not limited by the 1/3 bound given by the (equilibrium) KTHNY theory.

We rationalize our findings using linear elastic theory and show the existence of two well-defined effective temperatures quantifying respectively large-scale deformations and bond-order fluctuations. We argue that the root of these phenomena lies in the sole time-persistence of the effective noise felt by particles. They should thus be observed in many different situations, a few of which we discuss.

ON CURVATURE DEPENDENT INTERACTION BETWEEN MEMBRANE CHANNELS AND LIPID BILAYER

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Membrane channels are in lipid bilayer embedded proteins that play important roles in a variety of cellular processes. Their function may depend on membrane curvature at their location, and a possible reason for this could be their curvature dependent interaction with the lipid bilayer [1]. Such an interaction can be at a macroscopic level expressed in terms of the mismatch between the intrinsic principal curvatures of membrane inclusion and those of the membrane [2]. The corresponding expression involves two parameters which measure the interaction strength and can be considered to represent the intermediate level between system´s interatomic interactions and its macroscopic behavior. With respect to the latter it has been for example theoretically revealed that curvature dependent inclusion – lipid bilayer interaction causes a mutual effect on each other of membrane shape and lateral distribution of movable inclusions [3].

Here we shall first illustrate the utility of applying the described macroscopic expression for the inclusion – lipid bilayer interaction in the interpretation of measured curvature induced sorting of potassium channel KvAP [4]. Then it will be shown how this expression helped to explain the mechanism of action of the cation channel Piezo1 in the regulation of the red blood cell (RBC) volume [5]. In the proposed model it was predicted that, due to its intrinsic curvature, Piezo1 accumulates in the dimple regions of RBC discocyte shape. This prediction was subsequently confirmed experimentally [6, 7]. It will be revealed how it is possible on the basis of measured lateral distribution of Piezo1 to quantify also its effect on the RBC shape [8]. Finally, we shall also display a recently developed promising way to learn more about of the Piezo1 – lipid bilayer curvature dependent interaction from shapes of lipid vesicles containing a single Piezo1 molecule [9].

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EXTREME MECHANICS OF POLLEN DEFORMATION

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Pollen grains contain male plant genetic material encapsulated in a hard protective shell. In addition to hard parts, shell also consists of flexible, soft regions—apertures. Thanks to the design and distribution of the apertures, many pollen grains can fold in (infold) upon dehydration, protecting thus a sensitive interior. This mechanical design, however, may also lead to bursting of the apertures and the leakage of the pollen proteins in the atmosphere. Infolding pathways of pollen grains are investigated by studying elastic deformations of inhomogeneous thin shells. Different pathways are governed by the interplay between the elastic properties of the hard and soft regions of the pollen shell and by the aperture shape, number, and size. The regions of mechanical parameters of the pollen grain which lead to complete closure of all apertures, thus reducing water loss and presenting viable solutions to the infolding problem are delineated [1]. The bursting of the grain once it swells enough in humid atmosphere is shown to be a rapid transition at the critical point when the aperture can no longer sustain the internal pressure [2].

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FROM SOLID STATE TO SOFT MATTER PHYSICS: STRUCTURAL DYNAMICS OF DNA EXPLORED BY DIELECTRIC AND INFRARED SPECTROSCOPY

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The aim of my talk is to show how tools from Solid State Physics, such as dielectric and infrared spectroscopy, can be applied to study structural dynamics in Soft Matter and Biological Physics. I will try to offer a fresh perspective on the research conducted in collaboration with Rudi since 2002 when we met in NIH, Bethesda for the first time. I will highlight some unique insights in the collective and single chain structural dynamics of DNA and show how these properties change in the function of DNA concentration, length and environment. I will discuss the roles of intrinsic DNA counterions and ions from the added salt in ionic screening, integrity of double stranded DNA form in pure water solutions and on highly hydrated thin films, as well as the nature of cation-mediated interactions. The obtained results provide additional understanding of DNA properties in the biological milieu despite the experimental conditions are usually far from physiological ones [1-7].

Working in the field of Biological Physics I have enjoyed fruitful collaboration and numerous discussions with colleagues and students whom I want to thank very much. In particular, I would like to mention Sanja Dolanski Babić, Lorena Griparić, Tomislav Ivek, Marko Pinterić and Tomislav Vuletić. Last but not least, my thanks go to Rudi Podgornik – virtuoso of Soft Matter – who deepened my interest and understanding of the subject and whose knowledge, wisdom and physical insight helped shape the experiments, as well as many thoughts that have gone into our papers.

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FROM KINETOPLAST DNA TO BIO-INSPIRED TOPOLOGICAL SUPRAMOLECULAR MATERIALS AND BACK

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Supramolecular materials built of topologically interlocked polymer rings have recently gained considerable interest in supramolecular chemistry, biology, and soft matter. Two typical exaples are polycatenanes, linear chains of concatenated rings, and the kinetoplast DNA (kDNA), the mitochondrial genome of trypanosomatids, formed by ~5000 dsDNA minirings linked together to form a 2D surface whose topology is on average conserved through replication. Here I present the results of several ongoing collaborative efforts, all highlighting the role of topological interactions in shaping the physical properties of supramolecular objects and how one can exploit them to tune the behavior of bioinspired materials. I will show that a relation *Twist*+*Writhe* = *constant*, typical of dsDNA rings, holds for circular polycatenanes, and that a similar effect holds for 2D sheets of rings. Finally, I will report the results of AFM measures of the kDNA, show how coarse-grained (CG) simulations of this system can be used to estimate the average linking number of the network, and how one can use CG simulations to explain the origin of the typical buckled shape of kDNA in solution. Our results suggest that supramolecular topological objects can form a new category of highly designable structures with potential applications in supramolecular chemistry and material science.

[1] L. Tubiana, F. Ferrari, andE. Orlandini, Phys. Rev. Lett. **129**, 227801 (2022).
[2] P. He, A. Katan, L. Tubiana, C. Dekker, and D. Michieletto, Phys. Rev. X in press (2023); bioRxiv (2022): 2022-09.

VIRUS SYMMETRY-BREAKING, ELASTICITY AND SELF-ASSEMBLY

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Spherical crystals are elementary models of geometric frustration in materials, with important realizations in a range of systems from viral shells and fullerenes to particle- and molecular-coated droplets. Using continuum elasticity theory, we study the structure and elastic energy of ground states of crystalline caps conforming to a spherical surface. We find that the ground states consist of positive disclination defects and that the ground states with icosahedral subgroup symmetries in caps arise across a range of curvatures, even far from the closure point of complete shells. Furthermore, we use Monte Carlo simulations to investigate the kinetic pathway of the formation of viral shells (capsids) and find that the key to the formation of perfect icosahedral capsids is in the strength of elastic energy compared to the protein-protein interactions and the chemical potential of free subunits. At the end of the talk, I will also discuss our ongoing efforts to understand the formation of SARS-CoV-2 particles within host cells. Unlike icosahedral viruses, the structures of coronaviruses are heterogeneous both in morphology and size, which greatly complicates the development of a theory regarding their formation.

At the end of the talk, I will also discuss our efforts to understand the formation of SARS-CoV-2 particles in their host cells. In contrast to icosahedral viruses, the structures of coronaviruses are heterogeneous both in morphology and size, significantly complicating any theory of their formation [1,2].

[1] S. Li and R. Zandi, Viruses **14**, 2089 (2022).
[2] R. Zandi, B. Dragnea, A. Travesset, and R. Podgornik, Phys. Rep. **847**, 1 (2020).

RNA ADSORPTION ONTO FLAT AND MEMBRANOUS SUBSTRATES FROM MULTISCALE MODELS

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RNA is a functionally rich biomolecule with multilevel, hierarchical structures whose role in the adsorption to molecular substrates is only beginning to be elucidated. Here, we use a multiscale strategy to first estimate the electrostatic interaction of the polyelectrolyte at a tractable coarse-grained level, which captures the fundamental electrostatic interaction in the adsorption processes onto a featureless charged substrate. Our results, indicating a selectivity in adsorption between single- and double-stranded regions of RNA, underline the importance of the RNA structure in regulating its adsorption to various substrates. We expect that the selective adsorption of one RNA structure over the other could be experimentally controlled by tuning the interaction strength, for instance, by changing the composition of lipid membranous substrates. Consequently, we tackle 5 different membrane compositions with all-atom models to obtain a finer resolution into the structural configurations of the RNA molecules during adsorption. The comparison of those RNA-membrane models interacting with an RNA (in "bulk water") provides several criteria of structural stability of the short RNA molecules influenced by a precise combination of lipids groups. Finally, we describe how these methods could contribute to a high-throughput design of effective lipid nanoparticles.