



UNIVERSITY
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Department of Physics



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March 17-20, 2019

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Book of abstracts

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Part I

Programme

Sunday, 17 March

16.00

OPENING
Uli Buchenau

Chairman: Giulio Monaco

16.15

From in-silico intuitions to experimental realizations with limited-valence DNA-made nanoparticles

Francesco Sciortino

16.35

Non-equilibrium phase transitions in driven Brownian motion

Philipp Maass

16.55

Heterogeneous local order in soft matter systems studied by X-ray cross correlation methods

Felix Lehmkuhler

17.15

Phase behaviour and rheology of multi-responsive soft microgels

Roberta Angelini

17.30

Anomalous Dynamics of Concentrated Silica-PNIPAm Nanogels

Lara Frenzel

17.45 - 18.15

COFFEE BREAK

Chairman: Walter Kob

18.15

Structure and dynamics of ionic liquids and other highly concentrated electrolytes

Aleksandar Matic

18.35

The fate of an ionic liquid confined in a nanopore

Stefano Mossa

18.55

Learning Transmission Matrices in Complex and Random Media

Luca Leuzzi

19.15

Anomalous transport in soft percolating host structures

Charlotte Petersen

19.30

Influence of deposition temperature and impurities on the refractive indices of thin films of methanol and ethanol

Dmitriy Sokolov

20.15

DINNER

21.15

POSTER SESSION

Monday, 18 March

Morning

Chairman: Uli Buchenau

8.30

How universal are "universal" anomalous properties of glasses at low temperatures?

Miguel Angel Ramos

8.50

Multi-scale relaxation in aging gels: from localized plastic events to system-spanning "quakes"

Roberto Piazza

9.10

Interference between the glass, gel, and gas-liquid transitions

Magdaleno Medina-Noyola

9.30

Short-time dynamics of confined colloids probed by high-energy coherent X-rays

Federico Zontone

9:45

Influence of wall heterogeneity on polymer nano-sandwiches

Raffaele Pastore

10.00

Measuring intensity correlation length in the bulk of a strongly scattering material

Marco Leonetti

10.15 - 10.45

COFFEE BREAK

Chairman: Josep Lluís Tamarit

10.45

On the structure of liquids: More order than expected

Walter Kob

11.05

A microscopic picture of the atomic motion during polyamorphism in an ultra-viscous liquid

Beatrice Ruta

11.25

Connecting dynamics and structure in disordered materials with machine learning

Tristan A. Sharp

11.45

Vitrification kinetics versus atomic mobility in a metallic glass former

Isabella Gallino

12.00

Origin of the X-ray beam induced dynamics in oxide glasses

Francesco Dallari

12.15

Breakdown of the Arrhenius Law in the Normal Liquid State

Andrzej Grzybowski

12.30 – 16.00

LUNCH BREAK

Afternoon

Chairman: Simone Capaccioli

16.00

The yielding transition of soft colloids

Luca Cipelletti

16.20

Dynamical behaviour of soft IPN microgels

Barbara Ruzicka

16.40

Long-wavelength fluctuations and anomalous breakdown of the Stokes-Einstein relation in two dimensions

Massimo Pica Ciamarra

17.00

Evidence of a low temperature dynamical transition in concentrated microgels

Marco Zanatta

17.15

The microscopic role of deformation in the dynamics of soft colloids

Nicoletta Gnan

17.30

Microscopic pathways for stress relaxation in repulsive colloidal glasses

Alessandro Martinelli

17.45 - 18.05

COFFEE BREAK

Chairman: Alexander Chumakov

18.05

New understanding of collective modes and thermodynamics of the liquid and supercritical states

Kostya Trachenko

18.25

"Static" Shear-Elasticity in Liquids & Melts

Laurence Noirez

18.45

Origin of boson peak in ordered crystals and amorphous solids

Alessio Zaccone

19.05

Boson peak and fracton in glass and single crystal probed by terahertz spectroscopy

Tatsuya Mori

19.20

Low energy vibrations, thermal transport and anharmonicity in ordered and disorder solids

Giovanna D'Angelo

20.15

DINNER

21.15

POSTER SESSION

Tuesday, 19 March

Morning

Chairman: Stephen Elliott

8.30

Fluctuating elasticity fails to capture sound damping in glasses

Anaël Lemaître

8.50

The Glass Transition: Can new data shed light on which Interpretation we should believe?

Patrick C. Royall

9.10

Long-range stress correlations in viscoelastic and glass-forming fluids

Alexander Semenov

9.30

Elasticity of Colloidal Systems by Video Microscopy Method

Deniz Kaya

9.45

Glass transition in ultrastable glasses: Analyzing the bulk transformation.

Ana Vila-Costa

10.00

The Impact of the Dipole Moment on the Crystallization Tendency of the Van Der Waals Liquids

Kajetan Koperwas

10.15 - 10.45

COFFEE BREAK

Chairman: Giuseppe Carini

10.45

Investigating the Anomalous Properties of Pressure-Densified Glasses

Adam P. Holt

11.05

Pressure-induced densification of vitreous silica: insight from elastic properties

Benoit Rufflé

11.25

Reducing the atomic two-level tunneling states in dielectric thin films

Xiao Liu

11.45

Is glycerol a good fruit fly of the glass community?

Tina Hecksher

12.00

Anomalous Magnetism of Non-Magnetic Glasses

Giancarlo Jug

12.15

Self-Assembling of Lysozyme: Microscopic and Macroscopic investigations

Sara Catalini

12.30 - 16.30

LUNCH BREAK

Afternoon

Chairman: Kia L. Ngai

16.00

Glassy features in translationally-ordered low-temperature halomethane crystals

Josep Lluís Tamarit

16.20

A new complex system: alpha-iron

Aleksandr Chumakov

16.40

Non-hydrodynamic modes in collective dynamics of liquids

Taras Bryk

17.00

Experimental evidence for a state-point dependent density-scaling exponent of liquid dynamics

Alejandro Sanz

17.15

Rejuvenation of a polymer melt after shear thinning and thermal jumps

Andrea Giuntoli

17.30 - 17.50

COFFEE BREAK

Chairman: Emanuela Zaccarelli

17.50

Dynamic density shaping of photokinetic E. coli

Claudio Maggi

18.10

Inverse modeling bacterial growth

Andrea De Martino

18.30

Systematic and non-uniform coarse-graining of biomolecules

Raffaello Potestio

18.50

Effect of dilution in asymmetric recurrent neural networks

Edoardo Milanetti

19.05

Phase Transitions in the Self-Organization of Neural Rosettes

Giorgio Gosti

20.15

SOCIAL DINNER

Wednesday, 20 March

Morning

Chairman: Giancarlo Ruocco

8.30

Field-cycling NMR relaxometry: A powerful tool for studying viscous liquids and polymers

Ernst Rössler

8.50

Complex local and glass transition dynamics in PA12 studied by broadband dielectric spectroscopy – What can we learn from hydration experiments?

Michael Wübbenhorst

9.10

Caged dynamics below the glass transition: connection to JG beta-relaxation

Simone Capaccioli

9.30

Watching structural dynamics in complex systems by tunable UV Resonant Raman scattering: from liquids to bio-systems

Barbara Rossi

9:45

Multimodal character of shear viscosity response in some hydrogen bonded liquids

Silvia Arrese-Igor

10:00

Deviations of dynamic parameters in glass forming alkyl phosphates

Manoj Kumar Saini

10.15 – 10.45

COFFEE BREAK

Chairman: Luca Leuzzi

10.45

Simulation of structural relaxation and glass transitions in d-sorbitol

Stephen R. Elliott

11.05

Toward better understanding of the density scaling law

Marian Paluch

11.25

Glass Transition and Lack of Equipartition in a Statistical Mechanics model of Random Lasers

Giacomo Gradenigo

11.45

Laser Induced Nucleation in Supersaturated Aqueous KCl Solutions

Renato Torre

12.05

A microscopic look at the Johari-Goldstein relaxation in a hydrogen-bonded liquid

Federico Caporaletti

12.20

Possible universal relation between short time β -relaxation and long time α -relaxation in glass-forming liquids

Rajsekhar Das

12.35 - 16.30

LUNCH BREAK

Afternoon

Chairman: Marian Paluch

16.00

Slow dynamics of supercooled hydration water in biosolutions

Paola Gallo

16.20

Kosmotrope and Chaotrope Salts Influence on Water Structural Relaxation and hydrogen Bond Dynamics Investigated by Coherent Quasielastic Neutron Scattering

Antonio Faraone

16.40

Liquid and Solid Polyamorphism of Water: Recent Simulations and Experiments

Philip H. Handle

17.00

Reduced dielectric response of water on the nanoscale

Jasper Schmidt Hansen

17.15

Dynamics of water and related H-bonded liquids

Catalin Gainaru

17.30

Hydrogen order and disorder in a high-pressure phase of H₂O ice: Ice VI

Tobias M. Gasser

17.45

CONCLUSIVE REMARKS

Kia L. Ngai

Part II

Talks

PHASE BEHAVIOUR AND RHEOLOGY OF MULTI-RESPONSIVE SOFT MICROGELS

R. Angelini^{1,2}, V. Nigro^{1,2}, B. Ruzicka^{1,2}, E. Zaccarelli^{1,2}

¹Istituto dei Sistemi Complessi del Consiglio Nazionale delle Ricerche (ISC-CNR), UOS Sapienza, Roma, 00185, Italy.

²Dipartimento di Fisica, Sapienza Università di Roma, Roma, 00185, Italy.

Multi-responsive microgels are widely studied hybrid systems that combine the properties of polymers and colloids. Due to their complex morphology, the microscopic interactions and consequently the viscoelastic properties of these soft particles are still not completely understood. Combining differential scanning calorimetry and rheometry, we investigate a thermo- and pH-sensitive microgel composed of Interpenetrated Polymer Network (IPN) of poly(N-isopropylacrylamide) (PNIPAM) and poly(acrylic acid) (PAAc). These particles are characterized by topological inhomogeneities due to their crosslinking degree and to the PNIPAM/PAAc ratio [1] that strongly affect their elasticity and viscoelastic behaviour. The frequency dependent linear viscoelastic properties across the typical swollen-shrunk volume phase transition [2] are here deeply investigated depending on concentration, pH and PAAc.

[1] V. Nigro *et al.*, *J. of Chem. Phys.* **143**, 114904 (2015).

[2] V. Nigro *et al.*, *Soft Matter* **13**, 5185 (2017).

MULTIMODAL CHARACTER OF SHEAR VISCOSITY RESPONSE IN SOME HYDROGEN BONDED LIQUIDS

S. Arrese-Igor¹, A. Alegria^{1,2}, J. Colmenero^{1,2,3}

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²Departamento de Física de Materiales UPV/EHU, Apartado 1072, 20080 San Sebastián, Spain.

³Donostia International Physics Center DIPC, Paseo Manuel Lardizabal 4, 20018 San Sebastián, Spain.

Shear viscosity is a transport property of liquids determined by dynamics and measuring the resistance of the liquid to flow. Yet, it is not always obvious how the macroscopic flow is connected to the atomic/molecular dynamics and complex phenomena can emerge from the presence of different kinds and degrees of intermolecular interactions between molecules, which, in some cases, result in transient network structures and complicate the molecular scale picture of viscosity. Hydrogen bonding and Coulombic interactions for example are responsible for the mesoscopic structure arising in some monoalcohol and ionic liquids with long alkyl chains [1]. Here the impact of supramolecular aggregate formation on the shear viscosity response of hydrogen bonded liquids was investigated paying special attention to the complex viscosity representation. In particular, we studied the shear mechanical response of several monoalcohols showing exponential and non-exponential shape dielectric Debye-like relaxation [2]. In addition to the structural relaxation, distinctive of the glass transition, and the terminal crossover to pure viscous flow, characteristic of simple liquid flow, systematic analysis of complex viscosity curves evidences the presence of an additional intermediate process between those two.

[1] A. Perera, *Phys. Chem. Chem. Phys.*, **19**, 1062-1073 (2017).

[2] R. Böhmer, C. Gainaru and R. Richert, *Phys. Rep.*, **545**, 125-195 (2014).

NON-HYDRODYNAMIC MODES IN COLLECTIVE DYNAMICS OF LIQUIDS

T. Bryk^{1,2}, I. Mryglod¹, G. Ruocco^{3,4}

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²Lviv Polytechnic National University, Lviv UA-79013, Ukraine.

³Istituto Italiano di Tecnologia@Sapienza, Rome I-00161, Italy.

⁴Università di Roma La Sapienza, Rome I-00185, Italy.

We report analysis of collective dynamics of liquids by a combination of analytical approach and molecular dynamics simulations. The theory is based on a matrix representation of generalized Langevin equation constructed on the chosen basis of dynamic variables. The basis usually includes all the dynamic variables connected with conserved quantities as well as with the fluctuations of non-conserved collective quantities (like stress tensor fluctuations, thermal stress fluctuations etc). Analytical solutions of the matrix equation is obtained in terms of dynamic k -dependent eigenmodes $z_i(k)$, which are either pairs of complex-conjugated eigenvalues (propagating modes) or purely real eigenvalues representing relaxing modes. Among all the eigenmodes the ones with k^2 -dependent damping in the long-wavelength limit correspond to generalized hydrodynamic modes, while the others represent non-hydrodynamic relaxing and propagating processes in liquids.

We discuss analytical solutions for several liquids in a wide range of densities and compare them with simulation data. We show the implications of the dynamic eigenmode analysis for understanding the viscoelastic transition in fluids as well as the emergence of non-hydrodynamic shear and heat waves. In particular, the analytical solutions of the viscoelastic and thermo-viscoelastic dynamic models allow to identify the "positive sound dispersion" via first correction to the linear hydrodynamic dispersion law and find out the processes responsible for its emergence. A comparison with other approaches of analysis of viscoelastic transition will be made.

CAGED DYNAMICS BELOW THE GLASS TRANSITION: CONNECTION TO JG β -RELAXATION

S. Capaccioli¹, K.L. Ngai², G. Ciampalini¹, M. Pochetti³, A. Paciaroni⁴

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²CNR-IPCF, Largo B. Pontecorvo 3, 56127, Pisa, Italy.

³Department of Physics, University of Trieste, Via Valerio 2, 34127, Trieste, Italy.

⁴Dip. di Fisica, Università di Perugia, Via A. Pascoli 1, 06123 Perugia, Italy.

We report recent studies by neutron scattering and THz absorption on the fast dynamics (typically in the ns-ps range) of different classes of glass-formers: polyalcohols [1], amorphous polymers, van der Waals molecules, metallic alloys [2, 3]. In the glassy state the molecular caged dynamics (i.e. libration-vibration motions) appear in susceptibility losses as a frequency power law with a small exponent, before attaining the region where the vibrational density of states dominated by the microscopic peak. Remarkably, the caged dynamics amplitude appears strongly linked to slow dynamics, in particular to α - and β -relaxation revealed by calorimetry or dielectric spectroscopy: the fast caged dynamics intensity $A(T)$ changes temperature dependence around the secondary glass transition temperature $T_{g\beta}$ occurring when the Johari-Goldstein (JG) β -relaxation time reaches ~ 1 ks and, at higher temperature, at the glass transition T_g . This outstanding property follows as consequence of the density dependence of the caged dynamics and its coupling to the JG β -relaxation. The present study extends the generality of the property and its explanation to carbohydrates and solvated proteins. These results may improve the understanding of biopreservation of proteins when embedded in glassy matrices.

[1] S. Capaccioli *et al.*, J. Phys. Chem. B **119**, 8800 (2015).

[2] K.L. Ngai *et al.*, J. Phys. Chem. B **119**, 12502+12519 (2015).

[3] Z. Wang *et al.*, J. Appl. Phys. **119**, 024902 (2016).

A MICROSCOPIC LOOK AT THE JOHARI-GOLDSTEIN RELAXATION IN A HYDROGEN-BONDED LIQUID

F. Caporaletti¹, S. Capaccioli², S. Valenti³, M. Mikolasek⁴, A.I. Chumakov^{4,5} and G. Monaco¹

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²Physics Department, University of Pisa, Largo B. Pontecorvo 3, 56127, Pisa, Italy.

³Physics Department, Universitat Politècnica de Catalunya, C. Jordi Girona, 1-308034 Barcelona, Spain.

³Department of Physics, University of Trieste, Via Valerio 2, 34127, Trieste, Italy.

⁴ESRF, The European Synchrotron, 71 Avenue des Martyrs, F-38000 Grenoble, France.

⁵National Research Center "Kurchatov Institute", 123182 Moscow, Russia.

Understanding the glass transition requires getting the picture of the dynamical processes that intervene in it. Glass-forming liquids show a characteristic decoupling of relaxation processes when they are cooled down towards the glassy state. Two main relaxations can indeed be distinguished: the well known α -relaxation, directly related to the process of dynamic arrest, and the faster Johari-Goldstein or β -relaxation. This last one is still under scrutiny as it is strictly related to and act as a precursor of the α -relaxation [1]. Its full explanation is therefore crucial for a complete theory of the glass transition, and necessitates information at the microscopic scale. However, probing the molecular dynamics of this process when its timescale is well separated from that of the α -one (>1 ns) is extremely challenging both using simulations [2-3] and experimentally. To this aim, nuclear γ -resonance time domain interferometry (TDI) has been utilized to investigate 5-methyl-2-hexanol, a hydrogen-bonded liquid with a pronounced process as probed by dielectric spectroscopy [4]. TDI, indeed is one of the few techniques able to probe dynamics with characteristic times in the range 10 ns-10 μ s, that is in the time-range where the β -relaxation decouples from the α , at the Ångstrom length-scale [5-6]. Our measurements [7], spanning both inter- and intra-molecular distances, demonstrate that the β -relaxation consists of cooperative and spatially restricted rearrangements, and allow us to estimate its characteristic length-scale.

[1] S. Capaccioli *et al.*, J. Phys. Chem. Lett. **3**, 735 (2012).

[2] H.B. Yu *et al.*, Sci. Adv. **3**, 1701577(2017)

[3] D. Fragiadakis and C. M. Roland, Phys. Rev. E **86**, 020501(R) (2012).

[4] J. Gabriel *et al.*, Phys. Rev. Lett. **121**, 035501 (2018).

[5] M. Saito *et al.*, Phys. Rev. Lett. **109**, 115705 (2012).

[6] F. Caporaletti *et al.*, Rev. Sci. Instrum. **88**, 105114 (2017).

[7] F. Caporaletti *et al.*, in preparation.

SELF-ASSEMBLING OF LYSOZYME: MICROSCOPIC AND MACROSCOPIC INVESTIGATIONS

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⁴Elettra-Sincrotrone Trieste, Strada Statale 14 Km 163.5, Area Science 70 Park, 34149 Trieste, Italy.

⁵University of Camerino, School of Biosciences and Biotechnology, Camerino, Italy.

⁶School of Pharmacy University of Camerino, Camerino, Italy.

Proteins based hydrogel have recently received great attention thanks to their capability to retain inside the matrix up to 97% of water or biologic fluids, making these materials similar to live tissues. For the aforementioned reasons, recently hydrogels have been used as scaffolds for stem cells, showing how the specific mechanical properties of gel can modulate the differentiation processes. In particular, Lysozyme hydrogels are promising candidates to form successful cell scaffolds, thanks to their high cyto-compatibility. The structural and dynamic properties of Lysozyme hydrogels can be tuned by modifying the aggregation conditions. In fact, the aggregation processes are characterized by different steps in which the protein undergoes conformational rearrangements and intermolecular association to form stable structures of increasing complexity. The β -sheet motif appears to be deeply involved in the self-assembling processes and in the development of hydrogel networks. In this work, has been studied the unfolding, aggregation and gelation processes of highly concentrated solution of Lysozyme in denaturing conditions as a function of temperature. We investigate the protein structural modifications through Infrared and UV-Raman spectroscopies and the elastic-viscous-thermal proprieties by Transient Grating spectroscopy, with the aim to compare and link micro- and macro-observables of these promising materials.

A NEW COMPLEX SYSTEM: ALPHA-IRON

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²National Research Centre Kurchatov Institute; Moscow, Russia.

³Deutsches Elektronen Synchrotron; Hamburg, Germany.

⁴Advanced Photon Source, Argonne National Laboratory; Lemont, Illinois; USA.

Nuclear Resonance beamline at the ESRF recently offered to users a new type of instrument: Hard X-Ray Spectrograph. The device enables phonon spectroscopy with the energy resolution of $\sim 100 \mu\text{eV}$, while using all radiation components in a broad ($\sim \text{meV}$) spectral window. Thus, almost an order of magnitude improvement in the energy resolution is achieved without sacrificing intensity.

Already the first applications of the device seem to open new physics. Phonon spectroscopy of usual alpha-iron at ambient conditions shows that alpha-iron, possibly one of the best studied by mankind substance, is actually not a simple system. At very low ($\sim \text{meV}$) energy transfer, the reduced density of phonon states show a distinct elevation over the level of acoustic modes expected from sound velocities.

Additional experimental data show that this anomalous soft dynamics is intrinsic to an ideal iron lattice. It cannot be attributed to possible imperfections as impurities, grain boundaries, texture, and magnetic domains. It also is not an experimental artifact, because measurements of other systems do not show this feature.

Analyzing possible reasons of the effect, we note that positive dispersion of acoustic modes seems to be excluded by previously reported neutron studies. Possibly, the anomalous soft dynamics is caused by unharmonicity, as the effect is drastically enhanced by temperature.

THE YIELDING TRANSITION OF SOFT COLLOIDS

S. Aime^{1,2}, D. Truzzolillo¹, L. Ramos¹, L. Cipelletti¹

¹L2C University of Montpellier and CNRS, France.

²DEAS, Harvard University.

We investigate the yielding transition of dense suspensions of colloids interacting via a soft repulsive potential by simultaneously measuring their mechanical response and microscopic dynamics under an oscillating shear deformation. At low strain amplitude, the system exhibits ultraslow, ballistic dynamics characterized by a compressed exponential relaxation of correlators, similar to those reported for many jammed soft materials at rest.

Upon increasing the strain amplitude, the system undergoes a dynamic transition towards a steady state characterized by fast stretched exponential, diffusive-like relaxations. The dynamic transition coincides with the onset of the non-linear rheological response. While this scenario seems to be generic to soft colloids, the sharpness of the transition appears to depend on the potential details.

We present a simple model that accounts for this dynamic transition.

LOW ENERGY VIBRATIONS, THERMAL TRANSPORT AND ANHARMONICITY IN ORDERED AND DISORDER SOLIDS

G. D'Angelo¹

¹Dipartimento MIFT, Università di Messina, Messina, Italy and Istituto per i Processi Chimico-Fisici del C.N.R., Sez. di Messina, Italy.

In the last few years, there is an increasing number of evidences for glassy anomalies in vibrational and thermal properties of crystalline solids with minimal or no disorder.

Very recently, a new approach has been proposed by Baggioli and Zaccone [1] to explain the ubiquitous presence of boson peak in glasses and in disordered and ordered crystals. In this approach it is shown that the boson peak anomaly arises from the competition between acoustic propagating phonons and viscous damping.

In this talk the predictive validity of this model will be tested and compared with the experimental observations of vibrational dynamics and thermal conductivity of a plethora of ordered and disordered solids, emphasizing the role of the vibrational anharmonicity and the structural and defective disorder.

[1] M. Baggioli and A. Zaccone, arXiv:1810.09516 (2018).

ORIGIN OF THE X-RAY BEAM INDUCED DYNAMICS IN OXIDE GLASSES

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²University of Trento, via Sommarive 14, 38123 Povo (TN), Italy.

Wide-angle X-ray photon correlation (X-PCS) experiments have reported evidence of an unusually fast dynamics at the microscopic length scales in network glasses, well below the glass transition temperature [1]. It has been recognized that the origin of these unexpected movements is a reversible and non-destructive beam-induced effect [2]. The characteristic time of this induced dynamics is inversely proportional to the intensity of the X-ray beam with a coefficient that depends on the chemical composition and local structure of the probed glass [3,4], making it a potentially new tool to probe fundamental properties of a large group of disordered systems. Moreover, with the advent of extremely brilliant X-ray sources such as the fourth-generation synchrotron radiation facilities a complete knowledge of the x-ray - matter interactions has become of the utmost importance. However, the exact mechanisms behind this phenomenon are yet to be discovered, leaving room to several possible, and sometime contrasting, explanations.

I will discuss recent results from small angle x-ray scattering experiments revealing that this beam induced dynamics in the low q-limit bears strong similarities to stress relaxation processes in soft matter [5]. This observation supports the interpretation of the induced motions as primarily determined by the relaxation of internal microscopic stresses.

[1] B. Ruta *et al.*, Nat. Comm. **5**, 3939 (2014).

[2] B.Ruta *et al.*, Sci. Rep. **7**, 3962 (2017).

[3] G. Pintori, PhD thesis (2017).

[4] G.Pintori *et al.*, submitted.

[5] L.Cipelletti *et al.*, Phys. Rev. Lett. **84**, 2275 (2000).

POSSIBLE UNIVERSAL RELATION BETWEEN SHORT TIME β -RELAXATION AND LONG TIME α -RELAXATION IN GLASS-FORMING LIQUIDS

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Relaxation processes in supercooled liquids are known to exhibit interesting complex behavior. One of the hallmarks of this relaxation process observed in the measured auto correlation function is the occurrence of multiple steps of relaxations. The shorter time relaxation is known as the β -relaxation which is believed to be due to the motion of particles in the cage formed by their neighbors. The longer time relaxation is called the α -relaxation. The time scales of these two relaxation processes dramatically separate out with supercooling. In spite of decades of research, it is still not clearly known how these relaxation processes are related to each other. In this work, we show that there is a possible universal relation between short time β -relaxation and long time α -relaxation. We also show that the proposed relation can be rationalized within random first order transition theory of glass transition if power law relation is assumed between static and dynamic length scales.

INVERSE MODELING BACTERIAL GROWTH

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²CNR-NANOTEC, Institute of Nanotechnology, Rome UNIT (Italy).

We address the efficiency of growth in bacterial populations by an information-theoretic approach combining (1) the mean single-cell growth yield and (2) the amount of regulation required to achieve it. First, growth performance is found to be bounded by a theoretical "rate-distortion curve" linking the above quantities. Next, we show how values of (1) and (2) can be inferred, along with detailed reaction-level information, from mass spectrometry data probing experimental *E.coli* populations in different conditions. For a large number of experimental datasets, inferred points robustly approach the theoretical bound as the quality of the growth medium improves. On the other hand, by analysing the inferred behaviour of individual processes, we can characterize pathway usage and regulatory strength, highlighting how the interplay of gene expression and metabolism shapes growth properties. Our approach is fully scalable and yields information that is currently inaccessible by other methods, both in silico and experimental.

SIMULATION OF STRUCTURAL RELAXATION AND GLASS TRANSITIONS IN D-SORBITOL

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Molecular-dynamics (MD) simulations have been used to study liquid- and glassy-state dynamics, as well as α - and β -relaxation-related glass transitions, of the polyol, d-sorbitol ($C_6H_{14}O_6$), a canonical example of a hydrogen-bonded organic glass. A two-stage procedure was used, wherein ensembles of 12 d-sorbitol molecules were simulated. First, amorphous models were obtained using a reactive force-field (ReaxFF) potentials and a standard melt-and-quench procedure. These atomic configurations were then used for *ab initio* MD simulations, performed using the Vienna Ab-initio Simulation Package (VASP) to study the atomic dynamics. We have introduced a novel approach for exploring H-bond interactions between structural units in this system by using a novel 'dihedral-angle-rearrangement' indicator to shed light on the relaxation processes and dynamical heterogeneity. We find that both α - and β -relaxation processes are governed by cooperative and spatially-heterogeneous changes in H-bond dynamics that can be described by spatial- and dihedral-angle-rearrangement indicators. We have obtained clear evidence that the onset of β -relaxation is associated with an increase of molecular independence due to the sudden increase of hydroxyl-group H-atom mobility above the corresponding transition temperature, T_β , resulting in atomic-rattling motion within cage-like confined environments. In contrast, α -relaxation, dominating above the corresponding transition temperature, T_α , is related to the occurrence of molecules bonded to their surroundings by fewer than three H bonds at any given time, resulting in a further increase of molecular independence. The methodology used in, and the findings of, this study are of general applicability to other glass-forming systems.

KOSMOTROPE AND CHAOTROPE SALTS INFLUENCE ON WATER STRUCTURAL RELAXATION AND HYDROGEN BOND DYNAMICS INVESTIGATED BY COHERENT QUASIELASTIC NEUTRON SCATTERING

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Salts can either increase or decrease the solution viscosity when dissolved in water. This phenomenon has been traditionally interpreted within the classification of the solutes as kosmotropes (structure makers) and chaotropes (structure breakers), with reference to their hypothesized property of enhancing or weakening the hydrogen bond network. However, at the molecular level the distinction is less clear as both kosmotropes and chaotropes affect the structure of the surrounding water molecules. Using coherent quasielastic neutron scattering, we have investigated the structural dynamics of NaCl/D₂O and KCl/D₂O, NaCl being a kosmotrope and KCl being a chaotrope, respectively. By probing the dynamics of these systems at the structure factor peak, we measured how different salts affect the structural relaxation of water. At the same time, by collecting data at the second peak in the deuterium intermolecular partial structure factor, the hydrogen bond dynamics was probed. Whereas the hydrogen bonding dynamics is largely unchanged by the presence of the salts, NaCl and KCl affect the structural relaxation differently: the former slows down the dynamics whereas the latter mostly leaves the relaxation unchanged.

EFFECT OF DILUTION IN ASYMMETRIC RECURRENT NEURAL NETWORKS

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We numerically investigate the possible limit behaviors of synchronous discrete-time deterministic recurrent neural networks of N binary neurons as a function of a network's level of dilution and asymmetry. The network dilution measures the fraction of neuron pairs that are connected, and the network asymmetry measures to what extent the underlying connectivity matrix is asymmetric. We study the dynamical evolution of all the different initial conditions, thus characterizing the full dynamical landscape without imposing any learning rule. Because of the deterministic dynamics, each trajectory converges to an attractor, that can be either a fixed point or a limit cycle. These attractors form the set of all the possible limit behaviors of the neural network. We determine convergence times, limit cycles' lengths, number of attractors, and the sizes of the attractors' basin. Two network structures maximize the number of possible limit behaviors. The first optimal network structure is fully-connected and symmetric. On the contrary, the second optimal network structure is highly sparse and asymmetric. The latter optimal is similar to what observed in different biological neuronal circuits. These observations lead us to hypothesize that independently from any given learning model, an efficient and effective biologic network that stores a number of limit behaviors close to its maximum capacity tends to develop a connectivity structure similar to one of the optimal networks we found.

ANOMALOUS DYNAMICS OF CONCENTRATED SILICA-PNIPAM NANOGELS

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Poly(N-isopropylacrylamide) (PNIPAm) nanogels undergo a reversible volume phase transition (VPT) in water at a lower critical solution temperature (LCST) around 32°C, which results in a rapid collapse of the particle volume by increasing the temperature [1]. Beside technical and medical applications, it has become a frequently studied system in soft matter research as a model system to probe the specific phase behavior of soft colloids [2]. Via x-ray photon correlation spectroscopy (XPCS) and small angle x-ray scattering (SAXS) we investigate the structure and dynamics of highly concentrated PNIPAm core-shell nanogels around the LCST below the radiation damage threshold [3]. Here we studied the dynamics and interaction of the highly concentrated colloids ($w = 14.6$ wt %) as a function of temperature around the LCST as well as the modifications due to their reversible VPT. Upon heating from room temperature to 45°C we found three dynamical regimes: At low temperatures the colloids show a sub-diffusive, polymer driven dynamical behavior. Around the LCST the relaxation time decreases rapidly. For $T > 37^\circ\text{C}$ the dynamics slow down by more than three orders of magnitude and the particle motion becomes hyper-diffusive. Together with the static data, where we found indications of a transition from repulsive to attractive forces during the VPT, our results suggest a transition from a polymer-dominated liquid below the LCST to a jammed state at high temperatures and volume fractions.

[1] K. László *et al.*, *Soft Matter* **6**, 4335 (2010).

[2] P.S. Mohanty *et al.*, *J. Phys. Chem B* **112**, 14692 (2008).

[3] F. Lehmkuhler *et al.*, *IUCr* **6**, 801 (2018).

DYNAMICS OF WATER AND RELATED H-BONDED LIQUIDS

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Water exhibits a plethora of fascinating phenomena which continue to generate numerous controversies. Among them is the calorimetric and dielectric absorption of amorphous ices [1,2] under the dispute whether their underlying dynamics reflects liquid-like structural fluctuations (α -process) [3] or merely proton motion akin to crystalline ices [4,5]. On the other side of "no man's land", the microscopic mechanisms triggering the dielectric response of liquid water also remain highly debated. Once again, the question here is whether or not the main polarization process reflects the isotropic reorientation of water molecules associated with the α -process. Stimulated by the progress gained from the investigation of monohydroxy alcohols [6], a recently analysis based on dielectric spectroscopy, light scattering, and computer simulations was able to identify the dielectric fingerprints of water's α -dynamics [7]. In this presentation we will further highlight the similarities between the microscopic mechanisms generating the complex, yet similar relaxation pattern of water and alcohols. To this end we will introduce the Transient Tetrahedral Model of water as a companion approach to the Transient Chain Model discussed in relation to monohydroxy alcohols. We find that this model has the potential not only to describe the reach phenomenology of water above its melting point, but also to provide a resolution for the conflicting debate concerning the dynamics in glassy water.

[1] K. Amann-Winkel *et al.*, Proc. Nat. Acad. Sci. USA **44**, 17720 (2013).

[2] V. Fuentes Landete *et al.*, Phys. Rev. X **9**, in press.

[3] F. Perakis *et al.*, Proc. Natl. Acad. Sci. USA **114**, 8193 (2017).

[4] K. Amann-Winkel *et al.*, Rev. Mod. Phys. **88**, 011002 (2016).

[5] J. J. Shephard *et al.*, J. Phys. Chem. Lett. **8**, 1645 (2017).

[6] R. Böhmer *et al.*, R. Phys. Rep. **545**, 125 (2014).

[7] J.S. Hansen *et al.*, Phys. Rev. Lett. **116**, 237601 (2016).

VITRIFICATION KINETICS VERSUS ATOMIC MOBILITY IN A METALLIC GLASS FORMER

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Employing fast scanning calorimetry we characterized the atomic mobility related to the α -relaxation and the vitrification kinetics for a bulk metallic glass forming liquid [1]. The atomic mobility is assessed by means of a frequency dependent step response analysis, and compared with atomic dynamics based on dynamic mechanical spectroscopy [2] and x-ray photon correlation spectroscopy [3]. The vitrification kinetics is studied in terms of the cooling rate dependence of the limiting fictive temperature. The results challenge the conventional wisdom based on a one-to-one correlation between vitrification kinetics and the α -relaxation, and we show that these two aspects of the glassy dynamics are decoupled at relaxation time scales of greater than 0.1 s, corresponding to moderate cooling rates slower than 200 K/s. It results that the liquid vitrifies at a temperature that is lower than expected from the α -process. This separation is the more pronounced the more deeply the liquid is undercooled, which is in agreement with the scenario of a growing length scale for dynamic heterogeneities. The apparent reduction of the activation energy of the vitrification process is connected to multiple mechanisms involved in the relaxation of the glassy state, which are observed to exhibit mild Arrhenius temperature dependence [6]. The findings are in agreement with studies on non-metallic glass-formers [4-5] and suggest universality.

[1] X. Monnier *et al.*, in preparation (2019).

[2] Z. Evenson *et al.*, Phys. Rev. B **89**, 174204 (2014).

[3] S. Hechler *et al.*, Phys. Rev. Mat. **2**, 085603 (2018)

[4] X. Monnier and D. Cangialosi, Phys. Rev. Lett. **121**, 137801 (2018).

[5] M. Philipp *et al.*, Soft Matt. **14**, 3601 (2018).

[6] I. Gallino *et al.*, Acta Mat. **144**, 400 (2018).

SLOW DYNAMICS OF SUPERCOOLED HYDRATION WATER IN BIOSOLUTIONS

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I will show results from molecular dynamics simulations on the slow dynamics of hydration water in different biological solutions upon cooling. In all these solutions hydration water shows the presence of two different slow relaxations, each one with its dynamic crossovers upon cooling. One of the two relaxations is the α -relaxation related to water glassy behavior and present also in the bulk. The other one is characteristic only of hydration water, extremely slow, and it is coupled to the slow protein motions. I will more extensively focus on recent results of water and trehalose and I will show that for concentrations for which trehalose molecules form a cluster in the solution hydration water behaves upon cooling similar to protein hydration water. Trehalose clusters show a Trehalose Dynamical Transition (TDT) similar to the Protein Dynamical Transition (PDT). This TDT is also coupled to the long relaxation that shows a crossover from strong to strong [1] similar to protein hydration water. In the region of mild supercooling, before the well-known fragile to strong crossover takes place, the dynamics of the β and α relaxations of hydration water follows the predictions of the Mode Coupling Theory (MCT) [2].

[1] A. Iorio *et al.*, submitted.

[2] A. Iorio *et al.*, submitted.

HYDROGEN ORDER AND DISORDER IN A HIGH-PRESSURE PHASE OF H₂O ICE: ICE VI

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In the last twelve years, five new ice phases were experimentally prepared. Two of them are empty clathrate hydrates and three of them represent hydrogen ordered counterparts of previously known disordered ice phases. We report on hydrogen ordering in ice VI samples produced by cooling at pressures up to 2.00 GPa [1]. Based on results from calorimetry, dielectric relaxation spectroscopy, Raman spectroscopy, and powder X-ray diffraction the existence of a second hydrogen ordered polymorph related to ice VI was suggested. Powder X-ray data show the oxygen network to be the one of ice VI. For the 1.80 GPa sample the activation energy from dielectric spectroscopy is 45 kJ mol⁻¹, which is much larger than for the known hydrogen ordered proxy of ice VI, ice XV. Raman spectroscopy indicates the 1.80 GPa sample to be more ordered than ice XV. It is further distinct from ice XV in that it experiences hydrogen disordering above $\simeq 103$ K that is 26 K below the ice XV to ice VI disordering transition. Consequently, below 103 K it is thermodynamically more stable than ice XV, adding a stability region to the phase diagram of water. Hence, we refer to it as ice β -XV and characterized it to be more ordered than ice XV. In contrast, recent work [2] describes it as a deep glassy state related to ice VI. We will present data that help to distinguish between order and disorder in ices.

[1] T.M. Gasser *et al.*, Chem. Sci. **9**, 4224-4234 (2018).

[2] A. Rosu-Finsen *et al.*, Chem. Sci. **10**, 515-523 (2019).

REJUVENATION OF A POLYMER MELT AFTER SHEAR THINNING AND THERMAL JUMPS

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A broad range of glass forming liquids under steady shear deformation at a fixed shear rate $\dot{\gamma}$ exhibits shear thinning under this steady state condition. An effective shear viscosity $\eta(\dot{\gamma}) = \sigma/\dot{\gamma}$ can be defined and this quantity decreases progressively with increasing $\dot{\gamma}$, even for shear rates lower than the reciprocal structural relaxation time τ_α^{-1} . At high shear rates a power law decay $\eta(\dot{\gamma}) \sim \dot{\gamma}^{-\alpha}$ with α a non-universal constant is observed. If the shear is then abruptly stopped the system "rejuvenates", recovering its quiescent equilibrium properties on a time scale that depends on its τ_α . Despite the intrinsic theoretical interest and practical applications, among which industrial paintings and 3D printing, the topic is scarcely discussed in the literature. We present a computational study of the shear thinning and subsequent rejuvenation using a coarse grained polymer melt of unentangled chains. The evolution of the structural properties, dynamics and collective motion of the liquid during both the shear thinning and recovery are investigated and a comparison is made with the physical aging of glass forming liquids after a sudden thermal jump.

THE MICROSCOPIC ROLE OF DEFORMATION IN THE DYNAMICS OF SOFT COLLOIDS

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Unraveling the glass transition and jamming in soft colloidal systems remains a challenge for modern soft matter physics. An important open question is whether softness controls the dynamics in such dense conditions [1]. Numerical simulations represents a strong ally to elucidate this problem, but in most cases softness is tuned by modifying the pair-potential parameters allowing particles to overlap to a certain extent, while neglecting crucial aspects that contribute to the elastic properties of realistic particles. This makes the concept of "softness" in simulations and experiments very different. To fill this gap, I will discuss a new model of 2D polymer rings with tunable softness which undergo substantial deformation at high densities. The ability to deform has a strong impact on the dependence of the relaxation time on the packing fraction which change from fragile-to-strong. In addition, dynamics is controlled by an intermittent particle motion which gives rise to a compressed exponential decay of the self-intermediate scattering function. This behavior can be rationalized in terms of deformed rings that act as stress dipoles [2]. This simple model thus provides microscopic insights into two mechanisms which are of a deep interest in soft matter: the fragility dependence on softness and the occurrence of a compressed exponential decay in dynamical correlation functions [3].

[1] J. Mattsson *et al.*, *Nature* **462**, 83 (2009).

[2] L. Cipelletti *et al.*, *Phys. Rev. Lett.* **84**, 2275 (2000).

[3] N. Gnan *et al.*, arXiv:1806.04788.

PHASE TRANSITIONS IN THE SELF-ORGANIZATION OF NEURAL ROSETTES

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Neural rosettes are biological multi cellular structures that develop from the self-organization and differentiation of human induced Pluripotent Stem Cells (hiPSCs). This process models the emergence of the embryonic spinal cord primordium, the neural tube. Errors in the formation of the neural tube are the cause of two severe diseases, the spina bifida and anencephaly. While this phenomenon is recognized as an example of self-organization, we do not understand the fundamental mechanics that guides this process. An explanation based on stem cell differentiation lacks the ability to describe the emergence of spatial organization, and an explanation based on patterning models lacks the ability to explain how different groups of cells can collectively migrate and generate the neural tube. A truly interdisciplinary approach that combines stem cell biology, and active/soft matter physics is required to understand this process. We show that, a developing neural rosette can be modeled as an active material that undergoes a sequence of phase transitions. These phase transitions are the result of single cells' decisions which are encoded in the cells' DNA as responses to the cells' environment and external signals. We conclude that neural rosette development is a multi-scale self-organization process that involves both cell differentiation and tissue development. To understand rosette formation growth, migration, and cell type evolution must be understood together.

GLASS TRANSITION AND LACK OF EQUIPARTITION IN A STATISTICAL MECHANICS MODEL OF RANDOM LASERS

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The fluctuations in the emission spectra of Random Lasers can be understood in terms of a thermodynamic phase transition to a glassy phase: the amplitudes and phases of the electromagnetic field modes remain frozen in the same disordered configuration for the whole duration of the pulse.

So far the only analytical predictions on the thermodynamics of this "glassy phase of light" were obtained in the so-called narrow-band approximation. That is, all modes interacting with each other in a structureless (fully-connected) network where the mode frequencies play no role in the selection of interactions.

We present the numerical evidence, obtained from highly optimized simulations on graphic cards (GPU), that a glass transition of the Random First Order type is present in the system even when the interaction network of modes is created with a selection rule which takes into account frequencies. The model on such a correlated network, that we name "mode-locked" graph, better represents the topology of interactions of light modes in random laser experiments. Last, but not least, we show that on the mode locked graph the glass transition is concomitant with the breaking of energy equipartition between the fundamental degree of freedom of the system.

BREAKDOWN OF THE ARRHENIUS LAW IN THE NORMAL LIQUID STATE

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Since the end of the 19th century, the Arrhenius law has been considered as a standard rule valid for various physicochemical processes, including the thermodynamic evolution of dynamic quantities (primary relaxation time, viscosity, dc-conductivity) in the normal liquid state. Our recent studies show [1,2] that such a routine approach is actually improper to describe the temperature effect on relaxation dynamics of normal liquids in isobaric conditions (including those above the melting temperature at ambient pressure). This outcome is grounded in a successful application of the density scaling law to predict and describe the inflection point observed along isotherms measured at elevated pressures. If dynamic quantities are expressed by a function $f(\Gamma)$, where $\Gamma = \text{density}^\gamma/\text{temperature}$ and γ is a material constant [2], the inflection temperatures and pressures determine a dynamic crossover at $\Gamma = \Gamma_{infl}$. At $\Gamma > \Gamma_{infl}$, the super-Arrhenian cooperative dynamics occurs, which is characteristic of supercooled liquids, whereas $\Gamma < \Gamma_{infl}$ defines the fast dynamics region at high temperatures and low pressures at which the simple Arrhenius law is also broken. Both the regions can be consistently described by the density scaling based models [1,2].

[1] E. Thoms *et al.*, *J. Phys. Chem. Lett.* **9**, 1783 (2018).

[2] A. Grzybowski and M. Paluch, Universality of Density Scaling, in *The Scaling of Relaxation Processes*, F. Kremer, A. Loidl (Eds.), Springer Nature (2018).

LIQUID AND SOLID POLYAMORPHISM OF WATER: RECENT SIMULATIONS AND EXPERIMENTS

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It is a well known fact that water is a complex liquid. More than two decades ago computer simulations suggested that this complexity might stem from a low temperature liquid–liquid phase separation and an associated liquid–liquid critical point (LLCP). This suggestion resonated well with the apparent polyamorphism discovered in amorphous ices about a decade earlier. The LLCP-hypothesis is examined here using both computer simulations and experiments. Computer simulations are performed on both the supercooled equilibrium liquid and the amorphous ices using the TIP4P/2005 model of water. The simulation data are then analyzed using the potential energy landscape (PEL) formalism. It is found that the PEL quantities indicate the presence of an LLCP in this model [1]. PEL signatures related to phase transitions were also identified for the polyamorphic transitions of the TIP4P/2005 amorphous ices. Furthermore, the polyamorphic transition in the amorphous ices was studied experimentally. In situ volumetry and ex-situ x-ray diffraction also reveal sharp first-order like polyamorphic transitions [2] complementing the simulation results.

[1] P.H. Handle and F. Sciortino, *J. Chem. Phys.* **148**, 134505 (2018).

[2] P.H. Handle and T. Loerting, *J. Chem. Phys.* **148**, 124508 (2018).

REDUCED DIELECTRIC RESPONSE OF WATER ON THE NANOSCALE

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Understanding dynamical properties of fluids on the nano-scale gives fundamental new insight into the underlying processes in fluidic systems. In this talk I will discuss the nano-scale dielectric property of water. First, through molecular dynamics simulations it is shown that the dispersion relation for the dielectric spectrum is proportional to the wave-vector squared indicating that there exists an underlying diffusive process in the system [1,2]. Then by application of the microscopic hydrodynamic operator formalism [3] the dynamical equation for the polarization density is derived, and from this it is shown that diffusion of polarization can account for the observed phenomenon. This diffusion process significantly reduces the dielectric response of any dielectric material when the local electric field features nano-scale variation. Such a situation arises in nano-confinement and polarization diffusion should be included in the modeling of nano-scale lab-on-a-chip devices.

[1] J.S. Hansen, J. Chem. Phys. **143**, 194507 (2015).

[2] J.S. Hansen, Mol. Sim. **42**, 1364 (2016).

[3] J.S. Hansen *et al.* Langmuir **31**, 13275 (2015).

IS GLYCEROL A GOOD FRUIT FLY OF THE GLASS COMMUNITY?

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Glycerol is the preferred prototypical glass-forming substance for experimenters in the glass community when testing models or demonstrating new techniques; probably due to its excellent glass-forming ability and large signal in many experimental methods [1]. However, there is also an increasing awareness that we should think of different classes of liquids, some simple and some more complex, and it would be sensible to choose the "standard" liquid among the simple systems. Does glycerol belong to that class? Here, we discuss some recent results for glycerol [2,3] that point in different directions regarding this question. It has been shown that glycerol has a sub-alpha feature in the rheological response similar to that found in mono-alcohols [2]. This slow mode is interpreted as a polymer-like response of the hydrogen-bonded network and indicates a complex dynamical behavior. On the other hand, in another recent work we show that glycerol obey single-parameter aging [3], i.e., it conforms to a simple aging behavior. In the end, the answer depends on what which criteria we have for a good fruit fly and how we define simple.

[1] K. Niss and T. Hecksher, *J. Chem. Phys.* **149**, 230901 (2018).

[2] L.A. Roed *et al.*, under review.

[3] J.S. Hansen *et al.*, *Phys. Chem. Chem. Phys.* **20**, 1716 (2018).

INVESTIGATING THE ANOMALOUS PROPERTIES OF PRESSURE-DENSIFIED GLASSES

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The nature of a glass is dependent on the temperature and pressure during its formation. Thus, "pressure densification", wherein a glass is formed at high pressure with the pressure subsequently released after vitrification, offers an opportunity to manipulate the physical properties of glasses. Experimentally it has been found that some molecular and polymeric glass formers pressure-densify to a greater extent than others, exhibiting higher density, suppressed local density fluctuations, and higher energy conformations. We applied a variety of experiment methods, including calorimetry, dielectric relaxation, and wide-angle x-ray and neutron scattering, in combination with molecular dynamics simulations, to understand what governs the effect of pressure on the vitrification process. Of particular interest is the kinetic stability and physical aging of the non-equilibrated states of a pressure-densified glass.

[1] D. Fragiadakis and C.M. Roland, *J. Chem. Phys.* **147**, 084508 (2017).

[2] R. Casalini, C.M. Roland, *J. Non-Cryst. Solids* **475**, 25 (2017).

[3] R. Casalini, C.M. Roland, *J. Chem. Phys.* **147**, 091104 (2017).

ANOMALOUS MAGNETISM OF NON-MAGNETIC GLASSES

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Non-magnetic glasses like the ubiquitous multi-component silicates normally don't display any relevant magnetic property in the measurement of the magnetization, M . A weak magnetization, of the order of some 10^{-4} to 10^{-1} emu/g, can nevertheless be measured at high values of H/T in a SQUID magnetometer and is normally ascribed to paramagnetic impurities (mostly Fe^{2+} for green glasses). Indeed, the SQUID-magnetization M is a standard mean of assessing the (nominal) Fe-concentration in these ordinary glasses.

However, we [1] have pointed out in 2015 that the nominal SQUID-concentrations do not correctly explain the H and T dependence of the specific heat C_p in some of these silicate glasses at cryogenic ($T < 4$ K) temperatures and moderate ($H < 30$ kOe) magnetic fields. An extra contribution, due to magnetic-field sensitive anomalous tunneling systems (ATS), is present in the glasses due to their intermediate-range atomic structure and explains well both M and C_p data with a significantly lower-than-nominal Fe-concentration.

In this talk, the case for the oddly magnetic-field dependent ATS-contribution to M is re-proposed in glasses and preliminary new SQUID data [2] are discussed for a commercial BK7 borosilicate sample. The new data confirm that a naïve paramagnetic contribution would lead to an Fe-concentration higher than that extracted from mass-spectrometry analysis of the sample and, moreover, H -dependent. Resorting to an ATS-contribution again would provide a more rational explanation of all sets of data, thus confirming the proposed [3] cellular atomic organization of glasses at intermediate-range.

[1] S. Bonfanti and G. Jug, *J. Low-Temp. Phys.* **180**, 214–237 (2015)

[2] G. Jug, *et al.*, unpublished results (2018).

[3] G. Jug in *Modern Problems in Molecular Physics*, L.A. Bulavin and AV. Chalji (Eds), Springer-Books (2018).

ELASTICITY OF COLLOIDAL SYSTEMS BY VIDEO MICROSCOPY METHOD

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Colloidal systems can be used as model systems to atomic systems. Phases of matter like liquids, glasses and crystals can be produced in colloidal systems. If the colloid sizes are close to microns, the motion of the particles can be captured live under a light microscope. In this setup, the local dynamics of the system can be studied once images are captured by a camera system. Here we use temperature sensitive microgel colloidal particles and we form colloidal crystals. Once the positions of the particles with time are measured by image analysis, we quantify the elasticity of the crystal at different temperatures. Our result follows previous results [1] that although positional order of microgel crystal is high, heterogeneous fluctuations are observed in the system which can be classified as disordered crystals. The crystals show Boson peak in their density of states data, which is a signature of disordered system. Here we show the normal modes of the crystal and how disorder is quantified in the system.

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[1] D. Kaya *et al.*, Science 329, 656 (2010).

ON THE STRUCTURE OF LIQUIDS: MORE ORDER THAN EXPECTED

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The structure of liquids and glasses is usually characterized by means of the radial distribution function or the static structure factor. Computer simulations or confocal microscopy experiments on colloidal systems allow also to access the bond angle distributions or the local connectivity of the atoms. However, all these quantities are basically one-dimensional in nature and hence it is hard to infer from them the real three dimensional structure of amorphous systems. As a consequence the structure of liquids and glasses is usually considered to be boring for distances beyond the second/third nearest neighbor. In this talk I will show that this is not the case at all and that by considering simple three dimensional correlation functions one finds a surprisingly ordered arrangement of the particles even at significantly larger distances. This order grows quite quickly if the temperature is lowered, showing that amorphous systems are way more ordered than expected from the study of the usual two-point correlation functions.

THE IMPACT OF THE DIPOLE MOMENT ON THE CRYSTALLIZATION TENDENCY OF THE VAN DER WAALS LIQUIDS

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From the fundamental point of view, the shape of molecules, their masses, and interaction potential determine the thermodynamics, dynamics and structural properties of any kinds of real substances. Intuitively, the increase in the attractive intermolecular interactions should cause a decrease in glass forming ability and makes that system should crystallize easier. However, our very last experimental and theoretical studies reveal completely contrary behavior [1]. We present that the systems, which are characterized by stronger molecular attraction, easier omit the crystallization, and hence they are better glass formers. Our results indicate that the strength of the attractive forces affects the location of the nucleation and crystal growth rate maxima with respect to each other and the melting point. Considering the origin of the attractive intermolecular forces, which among others result from interactions between dipole moments of the molecules, we explain how the spatial orientation of the dipole moment (in relation to the selected axis of the molecule) influence on the glass forming ability of the substance. Additionally, we present that the increase in crystallization tendency caused by gain in the pressure is more evident for systems characterized by weaker intermolecular attraction [2].

[1] X. Leng *et al.*, *Sci. Rep.* **6**, 36934 (2016).

[2] K. Koperwas *et al.*, *Phys. Rev. B* **96**, 224106 (2017).

HETEROGENEOUS LOCAL ORDER IN SOFT MATTER SYSTEMS STUDIED BY X RAY CROSS CORRELATION METHODS

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Accessing structure beyond pair correlation functions is expected to shed light on various open questions in condensed matter physics such as the glass transition phenomenon and self-assembly processes. These phenomena are governed by the appearance of dynamical heterogeneities, suggested to be closely connected to spatial heterogeneities and believed to play a key role in the glass transition process. In order to measure such structural heterogeneities in scattering experiments, higher-order correlation functions have to be defined using e.g. the X-ray Cross Correlation Analysis (XCCA) technique. Here, we will discuss our recent XCCA results on colloidal films and crystals [1,2]. A special focus is set on the in-situ self-assembly of nanocrystals made of PbS [3] and structure of assembled films of gold nanoparticles coated with a soft poly(ethylene glycol)-based shell [4]. Depending on the initial concentration of gold nanoparticles, structurally heterogeneous films are formed with dominating four- and six-folds symmetry. The amplitude of order parameters indicates that a minimum sample amount is necessary to obtain well-ordered structures. This richness of information cannot be achieved by standard microscopy techniques that are commonly used to characterize such nanoscale systems.

[1] M.A. Schroer *et al.*, *Soft Matter* **11**, 5465 (2015)

[2] F. Lehmkuhler *et al.*, *J. Appl. Cryst.* **49**, 2046 (2016).

[3] I. Lokteva *et al.*, under review (2019).

[4] F. Lehmkuhler *et al.*, *IUCrJ* **5**, 354 (2018).

FLUCTUATING ELASTICITY FAILS TO CAPTURE SOUND DAMPING IN GLASSES

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The fluctuating elasticity (FE) model is today the only theoretical framework available to analyze low-temperature acoustic scattering in glasses. Although its existing formulations neglect the tensorial nature of elasticity and exclude long-range disorder correlations, this can be amended by constructing it as the long wavelength approximation of the elastic response of the discrete, atomistic, problem. We show that, the FE model then fails to capture the observed damping in two respects: (i) it misses the anomalous scaling, and predicts the standard Rayleigh law; (ii) it grossly underestimates the amplitude of scattering by about two orders of magnitude. This brings clear evidence that the small scale non-affine displacement fields, although not simply reducible to local defects, play a crucial role in acoustic wave scattering and hence cannot be ignored.

MEASURING INTENSITY CORRELATION LENGTH IN THE BULK OF A STRONGLY SCATTERING MATERIAL

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Properties of light intensity "in the bulk" of a strongly scattering medium with microscopic grain size, is of importance for a large set of applications ranging from deep in-vivo live imaging and diagnostics, to atmospheric and space investigation.

When coherent light illuminates a turbid medium, speckles (that are spatially disorganized maxima of light intensity with well-known statistical properties [1]) are found. The key property of the speckle patterns is the spatial correlation length of the intensity, S , i.e. the speckle average diameter [2].

Here we demonstrate that it is possible to extract information about the properties in the bulk of a scattering material by studying the statistical properties of the intensity emission from fluorophores entombed in the medium and separated by a known distance. The probability density function of the intensity, obtained upon random illumination with many different (and random) speckle patterns, is strongly dependent on the distance between the emitters and on the local value of the refractive index. In particular, if the two fluorophores are located at a distance higher than S , the speckle contrast drastically falls.

Our method may be employed to measure refractive index fluctuations and the properties of the electromagnetic field in the bulk of special metamaterials.

[1] J.W. Goodman, *Speckle phenomena in optics: theory and applications* (2007).

[2] R. Carminati *et al.*, *Phys. Rev. A* **81**, 053804 (2010).

LEARNING TRANSMISSION MATRICES IN COMPLEX AND RANDOM MEDIA

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Linear problems are largely used in a variety of research fields, among which the characterization of the signal transmission in disordered system. In particular, the non-trivial problem of the reconstruction of the transmission matrix of random media is one of the most stimulating challenges in the field of biomedical imaging [1,2]. Its knowledge makes any opaque layer a normal optical tool [3,4], capable of focusing or transmitting an image through disorder, turning the scattering into a beneficial feature exploitable to enhance resolution. Many studies have pursued the resolution to this problem, with different techniques [5-8], achieving light-focusing control or reconstructing images behind complex media. In the present work, we investigate how statistical inference can help improving the calculation of the whole transmission matrix in an arbitrarily complicated light-scrambling environment. We convert a generic linear input-output transmission problem into a statistical mechanical formulation and, based on pseudolikelihood maximization algorithms, we learn the coupling matrix via randomly sampling intensity realizations. In this talk we propose a new statistical framework, bridging linear regression and thermodynamical approaches to uncover insights from the scattering problem. Among a number of possible applications, the main interest of the biomedical imaging community is toward its measurement in a disordered multi-mode fiber transmission [9], that would open up their usage against the more fragile and expensive single-mode bundle fibers counterpart in endoscopic devices.

- [1] J. Bertolotti *et al.*, *Nature* **491**, 232 (2012).
- [2] I.M. Vellekoop *et al.*, *Nat. Photonics* **4**, 320 (2010).
- [3] I. Freund *et al.*, *Phys. Rev. Lett.* **61**, 2328 (1988).
- [4] I. Freund, *Physica A* **168**, 49 (1990).
- [5] S.M. Popoff *et al.*, *Phys. Rev. Lett.* **104**, 100601 (2010).
- [6] S.M. Popoff *et al.*, *New J. Phys.* **13**, 123021 (2011).
- [7] J. Yoon *et al.*, *Opt. Express*, **23**, 10158 (2015).
- [8] J. Carpenter *et al.*, *Opt. Express*, **22**, 96 (2014).
- [9] D.E. Boonjazer Flaes *et al.*, *Phys. Rev. Lett.* **120**, 233901 (2018).

REDUCING THE ATOMIC TWO-LEVEL TUNNELING STATES IN DIELECTRIC THIN FILMS

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Vapor-deposited amorphous dielectric thin films differ from glasses cooled from liquids in that their properties are open to manipulation by their deposition parameters. As a result, stable glasses that bypass millions of years worth of structural relaxation have been produced. It has also been demonstrated that it is possible to reduce the density of atomic two-level tunnelling states (TLS) in dielectric amorphous thin films. The TLS are ubiquitous in amorphous solids and glasses where atoms or groups of atoms can tunnel between adjacent metastable locations at low temperatures. TLS have been a major limit to the quantum coherence times in a variety of quantum systems, such as superconducting qubits in quantum computers and quantum repeaters in fiber-optic based quantum communication networks. TLS-induced thermal noise is also one of the main noise sources in the mirror coatings of the next generation gravitational wave detectors. In this work, we explore deposition parameter space of dielectric thin film materials in order to reduce or even remove the TLS. We vary the growth temperature, film thicknesses, deposition rates, and methods of deposition. TLS density of states are primarily accessed by low temperature internal friction measurements using a high-Q double-paddle oscillator upon which the thin films are deposited. So far, e-beam evaporated amorphous silicon (a-Si) deposited at 400°C still has the lowest TLS density, which is two orders of magnitude smaller than those deposited at room temperature. Reduction of TLS density by a factor of 5-10 has also been observed in sputtered a-Si, e-beam evaporated amorphous germanium (a-Ge) and sputtered amorphous aluminium oxide (a-Al₂O₃). As a-Al₂O₃ has a different covalent bonding configuration from those of a-Si and a-Ge, and is a more practical dielectric material that has been used in superconducting qubits, this reduction is encouraging. We will discuss the effectiveness of controlling the TLS density by deposition parameters in terms of surface mobility during deposition, covalent bonding, and medium range order of the thin films.

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NON-EQUILIBRIUM PHASE TRANSITIONS IN DRIVEN BROWNIAN MOTION

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Models of driven transport in one dimension are applied to describe such diverse phenomena as biopolymerization, molecular motor motion, flow of molecules through nanopores, and ion conduction along membrane channels. A simple lattice model, the asymmetric simple exclusion process (ASEP) appears as a basic building block in these driven diffusion systems and gives rise to a number of phase transitions [1–4]. However, the ASEP may not be a correct model for continuous space dynamics. We introduce a Brownian ASEP (BASEP) with overdamped Brownian dynamics [5], where hard spheres with diameter σ are driven by a constant drag force through a cosine potential with period λ . The character of non-equilibrium steady states in this BASEP is strikingly different from that in the ASEP. Compared to a system of non-interacting particles, the current is enhanced for small σ/λ ratios due to a barrier reduction effect. Larger σ/λ ratios lead to a suppression of the current because of blocking effects. Surprisingly, an exchange-symmetry effect causes the current-density relation to be identical to that of non-interacting particles for commensurable lengths $\sigma = n\lambda$, $n = 1, 2, \dots$. A behavior similar as for the ASEP is obtained only in a limited parameter regime. The current-density relation leads to phase diagrams of non-equilibrium steady states that change with varying σ/λ ratio and can exhibit up to five different phases.

[1] R.A. Blythe and M.R. Evans, *J. Phys. A* **40**, R333 (2007).

[2] M. Dierl *et al.*, *Phys. Rev. Lett.* **108**, 060603 (2012).

[3] M. Dierl *et al.*, *Phys. Rev. E* **87**, 062126 (2013).

[4] M. Dierl *et al.*, *Phys. Rev. Lett.* **112**, 150601 (2014).

[5] D. Lips *et al.*, *Phys. Rev. Lett.* **121**, 160601 (2018).

DYNAMIC DENSITY SHAPING OF PHOTOKINETIC E. COLI

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Many motile microorganisms react to environmental light cues with a variety of motility responses guiding cells towards better conditions for survival and growth. The use of spatial light modulators could help to elucidate the mechanisms of photo-movements while, at the same time, providing an efficient strategy to achieve spatial and temporal control of cell concentration. In this talk I will demonstrate that millions of bacteria, genetically modified to swim smoothly with a light controllable speed, can be arranged into complex and reconfigurable density patterns using a digital light projector [1]. Moreover, using this strategy, a homogeneous "sea" of freely swimming bacteria can be made to morph very rapidly between different complex shapes. I will also show how to model non-local effects arising from memory in light response and how these can be mitigated by a feedback control strategy resulting in the detailed "bacterial" reproduction of grayscale density images.

[1] G. Frangipane *et al.*, *eLife* **7**, e36608 (2018).

MICROSCOPIC PATHWAYS FOR STRESS RELAXATION IN REPULSIVE COLLOIDAL GLASSES

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Residual stresses are well-known companions of all glassy materials. In some cases, the presence of such stress fields can give rise to extreme physical properties, like for example in the historical case of prince Rupert's drops. However, the interplay among these stress fields and the microscopic dynamics is still an open research field. It is known that they are linked to the particle mobility at small length-scales in many different amorphous systems, e.g. metallic glasses [1], colloidal glasses or collapsing gels [2]. Typically, the residual stress field is randomly distributed across the sample volume, but what happens when it possesses a defined symmetry? Recent XPCS results obtained on a colloidal glass of repulsive silica nanoparticles dispersed in a water-lutidine 2.6 mixture are presented in this talk. We observed that even in this class of materials the residual stress field gives rise to a very rich phenomenology in the dynamical properties as the presence of compressed relaxation functions and ballistic dynamics. Moreover, we were able to characterize dynamical heterogeneities as a function of both lag time and exchanged wave-vector [3]. The picture which emerges is one where the macroscopic stress stored in this colloidal glass relaxes via the cooperative motion of groups of particles with a characteristic size of the order of ten particle diameters.

[1] B. Ruta *et al.*, Phys. Rev. Lett. **109**, 165701 (2012).

[2] A. Duri and L. Cipelletti, EPL **76**, 972-978 (2006).

[3] F. Dallari, PhD Thesis (2018).

STRUCTURE AND DYNAMICS OF IONIC LIQUIDS AND OTHER HIGHLY CONCENTRATED ELECTROLYTES

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Ionic liquids have been highlighted as safe electrolytes for next generation batteries. The attractiveness arises from intrinsic properties such as high ionic conductivity, low vapour pressure and electrochemical stability. However, ionic liquids are also of high interest from a more fundamental point of view. Being just made up of ions coulombic interactions naturally dominate, but due to the generally bulky nature of the constituent ions there is in most cases also a large contribution from van der Waals forces. These competing interactions result in structural heterogeneities on the nm-length made up of apolar and polar domains.

A very much related class of liquids are highly concentrated electrolytes where the concentrations of ions is so high, typically 5-10 molar but can be even higher, that all the solvent molecules are tied up in coordinating the ions. This situation leads to properties very similar to ionic liquids and as well to an increased structuring on nm-length scales. In this contribution we will discuss the connection between local coordination, nm-heterogeneities and the dynamics for both ionic liquids and highly concentrated electrolytes. Using Raman spectroscopy, small angle x-ray scattering, XPCS, neutron spectroscopy and computer modelling we can reveal the structure and the dynamics on the relevant length scales as a function of both temperature and pressure.

INTERFERENCE BETWEEN THE GLASS, GEL, AND GAS-LIQUID TRANSITIONS

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The kinetic perspective of the non-equilibrium self-consistent generalized Langevin equation (NE-SCGLE) theory of irreversible processes in liquids [1] is applied here to study the interference between the non-equilibrium glass and gel transitions, and the gas-liquid equilibrium phase transition, of "Lennard-Jones-like" liquids instantaneously quenched to a final temperature T_f lower than the spinodal temperature T_s . The results reveal an unexpectedly rich and complex kinetic scenario, that describes spinodal decomposition, gelation, glass transition, and their combinations, within a common first-principles microscopic theoretical framework [2]. Among the most dramatic experimentally-observed effects, described by our results is a "latency" time t_l characterizing an initial pseudo-equilibration, in which the dynamic arrest stays latent [3]. This latency time $t_l(T_f)$ depends on T_f and diverges as T_f approaches T_s from below. For deeper quenches the dynamics exhibits the two-step structural relaxation observed in the simulation of the non-equilibrium dynamics of suspensions of HS particles transiently bonded by cross-linking polymeric agents [4,5]. Our results associate this two-step structural relaxation with a predicted low-temperature gel-glass transition.

[1] P. E. Ramírez-González and M. Medina-Noyola, Phys. Rev. E **82**, 061503 (2010).

[2] J.M. Olais-Govea *et al.*, J. Chem Phys. **143**, 174505 (2015)

[3] H. Guo *et al.*, J. Chem. Phys. **135**, 154903 (2011).

[4] N. Khalil *et al.*, Soft Matter **10**, 4800 (2014).

[5] P. Chauduri *et al.*, J. Chem Phys. **142**, 174503 (2015).

BOSON PEAK AND FRACTON IN GLASS AND SINGLE CRYSTAL PROBED BY TERAHERTZ SPECTROSCOPY

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In disordered materials, the boson peak (BP) is observed in the terahertz region as a universal feature of atomic vibration [1]. The BP closely relates to the universal temperature behavior of thermal properties of glassy system which is one of the unsolved problems in glass physics. Meanwhile, for polymer glass, the so-called fracton [2] excitation will universally appear in the frequency range above the BP frequency, and it will be originated from the self-similar connectivity of structural units. Interestingly, some particular single crystals such as some thermoelectric materials [3,5] and pure relaxor materials [6], show the universal temperature dependence of thermal properties of glassy system. Those anomalous thermal properties are originated from the off-center rattling phonon modes which correspond to the BP of actual glassy materials [5]. In addition, the fracton in single crystal is observed in the pure relaxors [4,7], by the connection of the dipole-dipole moments having a fractal structure. In the presentation, we show how to detect these universal excitations by terahertz spectroscopy [8], and discuss the difference of behaviors of BP and fracton between actual glassy materials and single crystals.

- [1] T. Nakayama, Rep. Prog. Phys. **65**, 1195 (2002).
- [2] S. Alexander and R. Orach, J. Phys. Lett. **43**, 625 (1982).
- [3] T. Mori *et al.*, Phys. Rev. Lett. **106**, 015501 (2011).
- [4] A. Koreeda *et al.*, Phys. Rev. Lett. **109**, 197601 (2012).
- [5] T. Takabatake *et al.*, Rev. Mod. Phys. **86**, 669 (2014).
- [6] M. Tachibana and E. Takayama-Muromachi, Phys. Rev. B **79**, 100104(R) (2009).
- [7] S. Tsukada *et al.*, Sci. Rep. **7**, 17508 (2017).
- [8] M. Kabeya *et al.*, Phys. Rev. B **94**, 224204 (2016).

THE FATE OF AN IONIC LIQUID CONFINED IN A NANOPORE

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Ionic liquids are mixtures of cations and anions which stay liquid at room conditions, a feature making them potentially ideal electrolytes for energy storage and conversion technologies. In these applications (e.g., supercapacitors) ionic liquids are often used in contact with solid interfaces, or even constrained in pores whose size can be less than a nanometer. In such extreme environments the properties of matter are drastically modified compared to the bulk counterparts. In this context one can address a primary issue: Does the phase nature of an ionic liquid change when it is confined in pores of nanometric size? The simplicity of this question is misleading. Experiments which probe ionic liquids at the nanoscale, in fact, are extremely difficult and sometimes in mutual contradiction, failing so far to provide a generally accepted answer.

I have tackled this issue systematically by massive Molecular Dynamics simulation of a simple model ionic liquid confined in a slit pore[1]. In this talk I will discuss how, by appropriately tuning size and temperature of the latter, I have revealed unexplored phase modifications. For instance, following an increase of the confinement, I have observed the formation of ionic liquid-crystal structures, which unexpectedly transform into plain stable liquid states and subsequently freeze in new crystal phases, with a remarkable reentrant behavior.

I will also show how these changes reflect on the relative organization of the ions (charges) and on their dynamical state. I will finally build on the simulation results to provide a consistent general picture of these systems, by also involving in the discussion disparate very recent theoretical and experimental inspiring work.

[1] S. Mossa, *Phys. Rev. X* **8**, 031062 (2018).

"STATIC" SHEAR-ELASTICITY IN LIQUIDS & MELTS

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On the basis of a Maxwell gas model (1867), it has long been accepted that liquids exhibit (shear) elasticity at high solicitation frequencies (MHz or GHz) only. A century and a half later, the existence of a nearly "static" elasticity (0.1–10Hz) is revealed [1]. The "static" shear elasticity is identified at sub-millimeter scale, both on simple liquids and complex fluids (polymer melts, molecular glass formers, Van der Waals liquids, ionic liquids, H-bond liquids including liquid water) pointing out a probable generic character. Liquids would possess a weak but finite elastic threshold below which they exhibit a solid-like behavior. It will be shown on some examples how the elastic response and the usual viscous behavior are connected. Low frequency shear elasticity in liquids has profound implications on fluidic transport mechanisms and instabilities or thermodynamics. It enables the identification of novel liquid properties as flow induced cooling, spectacular mechano-optical conversions highlighting harmonic oscillator behaviours or coexistence of local temperatures near a wall [2]. From a theoretical point of view, low frequency shear elasticity challenges molecular approaches like the viscoelasticity theory, while cooling challenges the viscous friction heating. It opens the route to alternative models [4] predicting a length-scale dependence of viscoelastic parameters [3,5], revisiting the Frenkel zero-frequency shear elasticity assumption by introducing solid-like gap-based approach [5].

[1] L. Noirez and P. Baroni, *J. of Phys.: Cond. Matter* **24**, 372101 (2012).

[2] L. Noirez *et al.*, *Appl. Phys. Lett.* **110**, 213904 (2017).

[3] F. Volino, *Ann. Phys.* **22**, 1 (1997).

[4] A. Zaccone *et al.*, *Phys Rev B* **84**, 174119 (2011)

[5] K. Trachenko and VV Brazhkin, *Rep. Prog. Phys.* **79** 01650 (2016).

TOWARD BETTER UNDERSTANDING OF THE DENSITY SCALING LAW

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For over half a century till the present time a tremendous scientific effort has been made to understand the molecular dynamics behavior of supercooled liquids. Recently a considerable progress has been achieved in this area by developing the density scaling concept. It has been demonstrated experimentally for a large number of various glass-forming liquids and polymer melts that structural relaxation times measured measure as a function of both temperature and pressure can be scaled onto single curve for given system if they are plotted vs. new variable: TV^γ , where γ is a scaling exponent, T is temperature and V denotes specific volume. The significance of this experimental fact was particularly appreciated when it was demonstrated that γ can be related to the exponent: $m = 3\gamma$ of the repulsive part of $U_{IP_L}(r) = A_r r^{-m}$ of the effective short-range potential for intermolecular interactions. The same form of the intermolecular potential can be used to derive the equation of state for description of PVT data. Thus, the analysis of the experimentally measured PVT by this new equation state could be alternative method for determination of the value of γ . However, it turns out that the determined using this method value of γ is typically two times larger than one obtained from analysis of the relaxation time. The new approach to molecular dynamics simulations proposed by us has employed to solve this long standing problem. Our results show that the anisotropy of intermolecular interactions, which invariably occurs for real molecules, is the reason for the discrepancy.

INFLUENCE OF WALL HETEROGENEITY ON POLYMER NANO-SANDWICHES

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Many applications of polymeric materials involve their dynamics on rough or chemically heterogeneous surfaces. Examples include adhesion, friction and rubber reinforcement by fillers. Surface heterogeneities lead to significant differences with respect to smooth surfaces, but our understanding of their role remains incomplete. We recently investigated, via molecular dynamic simulations, a polymer melt confined between surfaces with increasing spatial correlation (patchiness) of weakly and strongly interacting sites [1]. In this talk, we show that major changes in the polymer relaxation dynamics occur on changing the typical size of the heterogeneities, while keeping constant the surface chemical composition. When the surface patchiness exceeds a certain threshold, a dramatic decoupling between diffusion and structural relaxation occurs, which resembles the Stokes-Einstein breakdown in glass forming materials. Surprisingly, these large dynamical effects are accompanied by minor structural modifications. Our work suggests that, by proper design of the solid walls, it is possible to tune major dynamic and mechanical changes in nanoscopically confined polymers, and highlights the importance of controlling not just the surface chemistry but also the surface morphology.

[1] R. Pastore *et al.*, *Phys. Chem. Chem. Phys.* **21**, 772 (2019).

ANOMALOUS TRANSPORT IN SOFT PERCOLATING HOST STRUCTURES

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Transport in heterogeneous crowded environments occurs in many situations, including inside of cells, in catalysts, and in porous rock during oil recovery. Both experimentally, and in simple models, the transport in complex crowded media can be subdiffusive. The origin of this anomalous diffusion has been explained theoretically for the paradigmatic Lorentz model. Here, a single particle moves with Newtonian dynamics through a random array of identical fixed obstacles. The moving particle has specular collisions with the obstacles. At the percolating density of the obstacles, the mean square displacement grows subdiffusively. We extend the Lorentz model towards realistic systems by relaxing the hard-exclusion interaction assumption, and find that the system exhibits a percolation transition dependent on the energy of the probe particle, and the dynamics remain anomalous at the percolation point.

MULTI-SCALE RELAXATION IN AGING GELS: FROM LOCALIZED PLASTIC EVENTS TO SYSTEM-SPANNING "QUAKES"

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Relaxation of internal stresses through a cascade of microscopic restructuring events is the hallmark of many materials, ranging from amorphous solids like glasses and gels to geological structures subjected to a persistent external load. By means of Photon Correlation Imaging, a recently developed technique blending the powers of scattering and imaging, we provide a spatially and temporally resolved survey of the restructuring and aging processes that spontaneously occur in physical gels originating from arrested phase separation. We show that the temporal dynamics is characterized by an intermittent sequence of spatially-localized "micro-quakes" that eventually lead to global rearrangements occurring at a rate that scales with the gel age. Notably, these dramatic upheavals of the gel structure are heralded by a progressive acceleration of the microscopic gel dynamics that originates from recognizable active spots and then spread at a large but finite speed through the gel. Within the 'slack' phase between two of these 'macro-quakes', the fluctuations of the degree of temporal correlation obey a non-Gaussian statistics described by a generalized logistic distribution. The evidence we obtained suggests a strong connection both with the stress relaxation processes taking place in earthquake sequences and with recently proposed self-organized oscillator mechanisms of crystal plasticity.

LONG-WAVELENGTH FLUCTUATIONS AND ANOMALOUS BREAKDOWN OF THE STOKES-EINSTEIN RELATION IN TWO DIMENSIONS

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According to the Stokes-Einstein (SE) relation the diffusion coefficient D and the relaxation time τ of liquids are inversely proportional. The breakdown of this proportionality is one of the hallmarks of the heterogeneous dynamics of supercooled liquids, where the coexistence of particles with anomalously large and small displacements leads to $D \propto \tau^{-k}$ with $k < 1$. Unexpectedly, it has been recently demonstrated that the SE relationship also breaks down in two dimensional high-temperature liquids, where the dynamics is not heterogeneous, but this time with $k > 1$. Why is so? Here we show that this breakdown reflects the existence of Mermin-Wagner long-wavelength fluctuations, by demonstrating that the SE relation is recovered when these fluctuations are appropriately filtered out. Our results clarify that Mermin-Wagner fluctuations, which are relevant in two dimensional crystal, amorphous solids and supercooled liquids, play a surprisingly relevant role in the high-temperature and/or low-density liquid phase.

SYSTEMATIC AND NON-UNIFORM COARSE-GRAINING OF BIOMOLECULES

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The recent advancements in computational power are enabling researchers to perform high-resolution (i.e. atomistic) simulations of ever larger systems, such as protein assemblies reaching several millions of atoms, over biologically meaningful ranges of timescales. Nonetheless, the need remains of developing simplified descriptions of biological macromolecules, which not only reduce the computational cost and allow the extension of the simulation's length and time scales, rather they also offer valuable insight in the physical properties of the system by pinpointing and highlighting the relevant features of the latter. In this talk I will provide a brief overview of some typical issues and solutions employed in the field of biologically oriented coarse-graining, and discuss the necessity of overcoming the conventional approaches that employ a uniform mapping from high to low resolution models.

HOW UNIVERSAL ARE "UNIVERSAL" ANOMALOUS PROPERTIES OF GLASSES AT LOW TEMPERATURES?

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Glasses (and other amorphous solids), are known to universally exhibit *anomalous* properties at low temperatures very different from their crystalline counterparts. Specifically, below 1-2 K the specific heat $C_p(T)$ of glasses shows a linear temperature dependence and the thermal conductivity $k(T)$ a quadratic dependence on temperature –in contrast with the expected cubic behavior of crystals following Debye’s theory–, that has been ascribed to the ubiquitous existence of tunneling two-level systems (TLS). Moreover, at a few K, $k(T)$ of glasses exhibits a *plateau* and the specific heat a broad peak in C_p/T^3 , which has been associated to an excess in the Debye-reduced vibrational density of states $g(\omega)/\omega^2$ (the "boson peak"). In the last decades, some disordered crystals such as *orientational glasses* (a.k.a. "glassy crystals"), obtained by quenching a plastic crystal phase, have been found to present the very same glassy features. Nevertheless, recent works are casting doubts about this *universality* of "glassy behavior". On the one hand, some genuine amorphous solids have been found to lack TLS at low temperatures, whereas some truly crystalline solids, devoid of orientational disorder, seem to exhibit those glassy features.

We will discuss this fascinating topic by presenting recent experiments on different molecular solids, both truly amorphous solids (toluene, ultrastable glasses...) and crystals with a minimal amount of disorder such as pentachloronitrobenzene or halomethanes $\text{CCl}_{4-n}\text{Br}_n$ crystals, aiming to shed light on this issue.

FIELD-CYCLING NMR RELAXOMETRY: A POWERFUL TOOL FOR STUDYING VISCOUS LIQUIDS AND POLYMERS

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With the availability of commercial field-cycling (FC) relaxometers since 1997 together with progress of home-built instruments, NMR relaxometry has gained new impetus as a method of investigating the dynamics in complex fluids. The method provides the frequency dependence (dispersion) of the spin-lattice relaxation rate which directly reflects the spectral density of the underlying motional process. The relaxation data may be transformed to the susceptibility representation which allows a direct comparison with the dielectric relaxation spectra. In the case of protons, due to the intra- and intermolecular origin of the magnetic dipolar interactions, relaxation dispersion reflects rotational as well as translational dynamics. The latter displays a universal low-frequencies dispersion law which allows determining the diffusion coefficient D_{trans} in addition to the rotational time constant. Thus, within a single experiment the ratio $D_{\text{trans}}/D_{\text{rot}}$ can be extracted and a more or less strong failure of the Stokes-Einstein-Debye relation can be accessed. In combination with dielectric data, associated liquids like glycerol and its mixtures with dimethyl sulfoxide are studied and the results are compared to those of non-associated liquids. – Sub-diffusive translation found in polymers is accessed by singling out the intermolecular relaxation via isotope dilution experiments. Applying frequency-temperature superposition, master curves are obtained like in rheology which extend over more than ten decades in frequency/time. Via Fourier transformation the segmental mean square displacement as a function of time is revealed disclosing characteristic power-law behavior. Likewise, information on reorientational dynamics is provided by the isolated intramolecular relaxation. Thereby, thorough testing of current polymer theories becomes possible. Finally, FC NMR complements neutron scattering experiments and becomes a method of molecular rheology.

WATCHING STRUCTURAL DYNAMICS IN COMPLEX SYSTEMS BY TUNABLE UV RESONANT RAMAN SCATTERING: FROM LIQUIDS TO BIO-SYSTEMS

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Raman spectroscopy has been demonstrated to be a non-destructive means to investigate the structural dynamics of a wide variety of complex systems, from liquids, gels and polymers up to bio-macromolecules. UV Resonant Raman (UVR) scattering is a powerful experimental approach taking advantage on the sensitivity and selectivity needed to incisively monitor specific chromospheres within the sample. In the past few years, there was a growing in the use of UVR especially for addressing open issues in biological field, thanks also to the advancements in laser technology and the development of high efficiency detectors for the entire UV-visible region. However, the conventional laser sources suffer from the limitation of providing fixed wavelength energies, while a tunable radiation source in the UV range allow to "map" the whole resonance landscape for matching with the best experimental conditions. Here we will present a newly developed UVR facility that exploits the tunability of synchrotron radiation source available at Elettra Sincrotrone Trieste. The setup available on IUVS@Elettra enables to perform UVR experiments with a fine tunable source in the range of excitation wavelengths 200-270 nm, resulting in an innovative spectroscopy facility for approaching open issues especially in the field of complex systems. Selected case studies will be discussed in order to show the useful of UVR method and the areas of interactions with other research interests.

THE GLASS TRANSITION: CAN NEW DATA SHED LIGHT ON WHICH INTERPRETATION WE SHOULD BELIEVE?

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Our understanding of the mechanism by which the viscosity of supercooled liquids increases by many decades is hampered by the difficulty in discriminating apparently incompatible theoretical approaches which provide equally good descriptions of experimental data: which theory should we believe? To address this, the challenge lies in equilibrating samples sufficiently high viscosity that the theories can be discriminated. Recently, considerable progress has been made, [1], largely supporting theories which imagine a *thermodynamic* origin of the glass transition – in contrast to a predominately *dynamic* origin [2,3]. Nevertheless, plenty of evidence in support of dynamic facilitation (which posits that the glass transition is driven by a dynamical phase transition) exists [4], which can be accessed in experiments [5]. Here we use obtain very deeply supercooled configurations in a model glassformer. Remarkably, the Kauzmann point where the *thermodynamic* theories suggest a phase transition lies at the same temperature as the lower critical point of the *dynamical* transition. Our findings may enable us to reconcile the competing interpretations of the glass transition [4].

[1] P. Royall *et al.*, *J. Phys.: Condens. Matter* **30**, 363001 (2018).

[2] F. Turci *et al.*, *Phys. Rev. Lett.* **118**, 215501 (2017).

[3] J.E. Hallett *et al.*, *Nat. Comms.* **9**, 3272 (2018).

[4] Turci *et al.* *Phys. Rev. X* **7**, 031028 (2017).

[5] R. Pinchaipat *et al.*, *Phys. Rev. Lett.* **119**, 028004 (2017).

PRESSURE-INDUCED DENSIFICATION OF VITREOUS SILICA: INSIGHT FROM ELASTIC PROPERTIES

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In situ high-pressure Brillouin light scattering experiments along loading-unloading paths are used to investigate the compressibility of vitreous silica. An accurate equation of state is obtained below 9 GPa using sound velocities corrected for dispersion. Conversely, huge inelastic effects are observed in the range 10–60 GPa, unveiling the reversible transformation from the fourfold-coordinated structure to the sixfold one. We find that the associated density changes fully correlate with the average Si coordination number. Decompression curves from above 20 GPa reveal abrupt backward coordination changes around 10–15 GPa and significant hysteresis. Further, contrary to common wisdom, the residual densification of recovered silica samples can be figured out from the pressure cycles.

A MICROSCOPIC PICTURE OF THE ATOMIC MOTION DURING POLYAMORPHISM IN AN ULTRA-VISCOUS LIQUID

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Many materials, ranging from monatomic liquids to molecular systems and metallic glasses show transitions between different amorphous phases whose origin is still unknown [1]. In glass-formers, polyamorphism appears related to kinetic properties of the liquids, still not direct evidence of this has been reported so far. We present here the microscopic evidence of a connection between a liquid-liquid transition (LLT) and a fragile-to-strong dynamical crossover between ultra-viscous metallic liquids. For this purpose, we merged state-of-the-art synchrotron techniques, like high-energy X-ray diffraction and X-ray Photon Correlation Spectroscopy, with an unconventional protocol consisting in a quasi-static cooling of a supercooled liquid. With this approach, we have been able to observe a polyamorphic transition between two liquid structures with different kinetics whose origin appears related to an ordering process not involving density changes [2]. The wave-vector dependence of the dynamics in the low temperature strong phase reveals a peculiar slow-down of the main relaxation process at the inter-particle distance, reminiscent of the de Gennes narrowing found in the frequency domain for simple liquids [3]. This behavior is accompanied by the occurrence of dynamical heterogeneities on faster times scales and suggests the existence of a peculiar mechanism of hopping of caged particles for the atomic motion.

[1] K. Murata & H. Tanaka, *Nat. Mat.* **11**, 436 (2012).

[2] S. Hechler *et al.* *Phys. Rev. Mat.* **2**, 085603 (2018).

[3] B. Ruta *et al.* submitted.

DYNAMICAL BEHAVIOUR OF SOFT IPN MICROGELS

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The novel class of responsive microgels has recently become very popular since their smart responsivity to external stimuli makes them very attractive for industrial applications and excellent model systems for exploring the exotic behaviours emerging in soft colloids due to their softness that allows to explore high density states well beyond random close packing. Interpenetration of polymer networks (IPN) of poly(Nisopropylacrylamide) (PNIPAM) and poly(acrylic acid) (PAAc) provides microgels with independent sensitivity to both temperature and pH. Notwithstanding the IPN microgel potentialities, knowledge of their behaviour from a fundamental point of view is still very limited. In this work the dynamics of PNIPAM-PAAc IPN microgels approaching the glass transition has been investigated through Dynamic Light Scattering and X-ray Photon Correlation Spectroscopy. The slowing down of the dynamics with increasing particle concentration shows an exponential increase of the relaxation time followed by a power law in the glassy state, that, together with a stretched to compressed transition, appear to be a general common feature of many different glass-formers. Interestingly softness of IPN microgel particles can be tuned through the mutual PNIPAM-PAAc network composition [1], allowing to modulate the system fragility and to observe a strong-to-fragile transition [2].

[1] V. Nigro *et al.*, arXiv:1707.08542.

[2] V. Nigro *et al.*, *Soft Matter* **13**, 5185 (2017).

DEVIATIONS OF DYNAMIC PARAMETERS IN GLASS FORMING ALKYL PHOSPHATES

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We study a series of trialkyl phosphate in the supercooled regime using calorimetric and dielectric measurements. The dielectric fragility index m_d and the stretching exponent β_d of the Kohlrausch-Williams-Watts correlation function are determined. Analyses of the enthalpic relaxation data by the Tool-Narayanaswamy-Moynihan-Hodge formalism yield the enthalpic fragility index m_H and stretching exponent β_H . The results are finding a departure of the dielectric fragility indexes from the enthalpic ones as the length of branch chain increases in the trialkyl phosphates. The large difference between m_d and m_H , as well as between β_d and β_H of tributyl phosphate (TBP) is remarkable. The results suggest that the enthalpic relaxation involving the motions of all parts of TBP is global, while the dielectric relaxation detects the local rotation, which might originate from the rotation of the polar core dipole. This is supported by the quite comparable fragility determined by viscosity and the enthalpic relaxation. Alternatively, the differences are interpreted by the formation of molecular self-assemblies. The Kirkwood correlation factor (g_k) calculated at low temperatures is consistent with this interpretation. The g_k is found to coincide at ~ 0.6 at glass transition temperature (T_g) for trialkyl phosphates. The enthalpic relaxation serving as the more fundamental relaxation relevant to the structural relaxation is confirmed.

EXPERIMENTAL EVIDENCE FOR A STATE-POINT DEPENDENT DENSITY-SCALING EXPONENT OF LIQUID DYNAMICS

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A large class of liquids obeys density scaling characterised by an exponent, which quantifies the relative roles of temperature and density for the dynamics [1]. The density-scaling exponent is often regarded as a material constant. We present, however, experimental evidence that the scaling exponent of liquid dynamics, γ , is state-point dependent for the glass-formers tetramethyl-tetraphenyl-trisiloxane (DC704) and 5-polyphenyl ether (5PPE). A method is proposed that from dynamic and thermodynamic properties at equilibrium estimates the value of γ at any state point of the pressure-temperature plane, both in the supercooled and the normal liquid regimes [2]. This new route is free of model assumptions and can be utilised for both glass- and non-glass-forming materials. We confirm that γ is generally state-point dependent by reanalyzing data of 20 metallic liquids and two model liquids.

[1] R. Casalini and C. M. Roland, Phys. Rev. E. **69**, 062501 (2004).

[2] A. Sanz *et al.*, arXiv:1807.11746v2.

FROM IN-SILICO INTUITIONS TO EXPERIMENTAL REALIZATIONS WITH LIMITED-VALENCE DNA-MADE NANOPARTICLES

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DNA oligomers can nowadays be assembled to produce a large variety of nanometric constructs, via a cascade of self-assembly processes, each one guided by the length of complementary sequences of distinct DNA strands. In the talk I will show that it is possible to build bulk quantities of DNA-made nanoparticles that closely match idealized colloids, transferring modern in-paper and in-silico intuitions into experimental realizations. I will show how unconventional collective behaviors, recently explored theoretically and numerically, can indeed be reproduced in the lab. Specifically I will discuss: (i) how to exploit limited valence interactions to suppress phase separation, enhancing the stability of the equilibrium gel phase [1-3]; (ii) how to exploit competing interactions to generate a material that is fluid both at high and at low temperatures and a solid-like disordered open network structure in between [3-6] and (iii) how to exploit bond-swap dynamics to create an all-DNA vitrimer[7-8].

[1] E. Bianchi *et al.*, *Phys. Rev. Lett.* **97**, 168301, (2006).

[2] S. Biffi *et al.*, *Proc. Nat. Acad. Science* **110**, 15633-15 (2013).

[3] S. Biffi *et al.*, *Soft Matter*, **11**, 3132 (2015).

[4] J. Fernandez-Castanon *et al.*, *Soft Matter* **14**, 6431-6438 (2018).

[5] S. Roldan-Vargas *et al.*, *Sci. Rep.* **3**, 2451 (2013).

[6] F. Bomboi *et al.*, *Nat. Commun.* **7**, 13191 (2016).

[7] F. Romano and F. Sciortino, *Phys. Rev. Letts.* **114**, 078104 (2015).

[8] J. Fernandez-Castanon *et al.*, *ACS Macro Lett.* **8**, 84 (2019).

LONG-RANGE STRESS CORRELATIONS IN VISCOELASTIC AND GLASS-FORMING FLUIDS

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Liquids are lacking long-range order; as a result their structural stress correlations are short-range in space. Simple liquids also show a very short-term memory leading to stress correlations that can be described by delta-functions in space-time. On the other hand, many liquids (like polymer systems or supercooled glass-forming fluids) show long-term structural relaxations and very long stress relaxation times. However, until very recently it was not recognized that long-term memory effects in viscoelastic liquids must lead to long-range spatial correlations of stress, stress increments and particle displacements. This talk will demonstrate that non-simultaneous correlations of the full stress in 2-dimensional systems must follow the $1/r^{-2}$ power law decay. I will discuss the role of finite compressibility in the transition from short-range structural correlations to the emerging long-range dynamical correlation effect, and the time-dependence of long-range stress correlations. A simple and rigorous physical argument showing why stress correlations in supercooled glass-forming liquids must be long-range and anisotropic will be then presented and used as a basis to elucidate important differences in the space/time behavior of the stress correlation functions in glass-forming liquids, crystalline solids and polymer gels.

RHEOLOGY OF GLASS-FORMING LIQUIDS AS A PROBE OF THE ENERGY LANDSCAPE

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Atomistic understanding of the dynamical slowdown and strong vs. fragile behavior of super-cooled liquids near glass transition remain one of the most intriguing and unsolved problem in condensed matter physics. Although several theoretical models have been proposed in the literature over the last decades to explain these phenomena, direct experimental tests of the validity and the relative merits of these models have remained rather scant. In this talk I will discuss the ongoing studies in our laboratory of the linear and non-linear rheological behavior of a variety of chalcogenide glass-forming liquids under oscillatory and steady shear. Experiments in the linear regime will be shown to provide important clues into the nature of the free energy landscape that controls the equilibrium dynamic properties of highly viscous liquids near glass transition, while those in the nonlinear regime will shed light on the modification of this landscape, that gives rise to phenomena such as shear thinning.

CONNECTING DYNAMICS AND STRUCTURE IN DISORDERED MATERIALS WITH MACHINE LEARNING

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Relaxation of a disordered material typically involves constituent particles changing neighbors or rearranging. These rearrangements are central to the response of the material, but it has been difficult to predict them from the disordered material structure. We use a straight-forward machine learning method and find that individual particles can be well-classified according to their propensity to rearrange (termed their "softness") based on the local instantaneous particle configuration. The method has been applied to a range of experimental materials ranging from colloids to granular disk packings and simulated materials ranging from atoms in poly-crystalline grains boundaries to cells in biological tissue models. Structural features that increase softness depend on the material and often can be identified naturally from the machine learning. Additionally, the framework has provided insights into differences between grain boundaries and bulk glasses, the dynamics of rearrangement avalanches in brittle solids, and the locations of T1-transitions in cell vertex models.

INFLUENCE OF DEPOSITION TEMPERATURE AND IMPURITIES ON THE REFRACTIVE INDICES OF THIN FILMS OF METHANOL AND ETHANOL

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Hydrogen-bonding interactions continue to attract extensive interests in a wide variety of fields, especially those the formation of assembly structures. Methanol, too, has been a frequent research subject because of its ability to form extended hydrogen-bond networks[4] as well as its importance as a common solvent, in practical applications including fuel cells and catalysis, and as an abundant species to consider in various astrophysical and aerosol settings [1]. Many of these studies aim for a molecular picture of the structures and behavior of methanol in a heterogeneous environment, to resolve the underlying mechanisms that take place at interfaces and are often different from the bulk phenomena [2]. This work presents the results of an experimental study of the temperature dependence and impurities of argon and nitrogen on the refractive indices of thin films of methanol and ethanol and of the structural transformations of these substances. Measurements were carried out using a two-beam laser interferometer [3] in the temperature range of 14–130 K. It was found that near the temperatures of structural transformations, the temperature dependence of the refractive index shows a clear non-monotonic behavior.

[1] P.A. Gerakines and R.L. Hudson, *Astrophys. J.* **805**, L20 (2015).

[2] X. He *et al.*, *J. Chem. Phys.* **145**, 171102 (2016).

[3] A. Drobyshev *et al.*, *Low Temp. Phys.* **43**, 724 (2017).

GLASSY FEATURES IN TRANSLATIONALLY-ORDERED LOW-TEMPERATURE HALOMETHANE CRYSTALS

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Here we study minimally disordered crystalline systems in which only a few degrees of freedom depart from a fully ordered state. The chosen systems are the series of halomethanes $\text{CBr}_n\text{Cl}_{4-n}$, $n = 0, 1, 2$. These materials exhibit a series of thermally induced solid-solid phase transitions that are attributed to the ability to thermally activate rotational degrees of freedom within the crystalline state. For $n = 1, 2$ the isomorphous low-temperature crystalline phase corresponds to a monoclinic $C2/c$ complex structure ($Z = 32$) in which dynamical disorder originates by the random occupancy of lattice sites occupied by Cl or Br atoms, unlike CCl_4 which will serve as a reference isomorphous structure despite the similar dynamics found by nuclear quadrupole resonance. The occupational disorder gives rise to reorientational dynamical processes associated with reorientational motions of the molecular dipole and thus, to a similar dynamics found in canonical or orientational glasses. We analyze one of the leading macroscopic properties characterizing the thermal anomalies found in glasses, the specific heat, as well as the characteristics of the low-frequency vibrational density of states, $g(\omega)$. Both typical reduced representations for C_p/T^3 and $g(\omega)/\omega^2$ reveal the existence of a hump deviating from the constant value predicted by the Debye theory below 10 K and around 2–4 meV, respectively. In addition, specific heat at low-temperature (below 2 K) shows the existence of the tunneling two-level systems. To unravel the microscopic nature of vibrational excitations giving rise to the Boson peak, we also performed DFT calculations for the reference CCl_4 system. Such DFT calculations for the CCl_4 case enables us to demonstrate that the broad peak arises from a piling up (at around 3–4 meV) of low-energy optical modes together with acoustic modes near the Brillouin-zone boundaries.

INFLUENCE OF DEPOSITION TEMPERATURE AND IMPURITIES ON THE REFRACTIVE INDICES OF THIN FILMS OF METHANOL AND ETHANOL

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The nature of mechanisms controlling the nucleation processes is still today one of more intriguing problem of the condensed matter physics. It has been ascribed to different causes, but its understanding is still far to be complete[1].

The nucleation in saturated solutions can be induced by a short laser pulse of high intensity [2]; a series of experimental studies have proved that this phenomenon occur in water solutions of very different nature, where the solutes can vary from simple salts to complex biological molecules [3]. Even if the NonPhotochemical Laser Induced Nucleation (NPLIN) is known from more than 20 years, several fundamental aspects of it remain open problems [4]. Nevertheless, the NPLIN enables the possibility to perform spectroscopic measurements during the first steps of crystal nucleation and growth, opening the harvesting of new valuable information on this elusive phenomena.

We performed an experimental investigation of the nucleation phenomena induced by a 25 ps infrared laser pulse in a supersaturated aqueous KCl solution. In particular, we developed an experimental set-up able to perform a very fast imaging (up to $5 \cdot 10^5$ frame/sec) of the solution modifications induced by the laser pulse. The fast imaging shows a series of physical processes taking place in the solution between the laser pulse arrival and the show up of the crystal nucleus.

[1] K.F. Kelton and D. Frenkel, *J. Chem. Phys.* **145**, 21 (2016).

[2] B.A. Garez *et al.*, *Phys. Rev. Lett.* **77**, 3475 (1996).

[3] W. Li *et al.*, *Cryst. Growth Des.* **16**, 2514 (2016).

[4] R. Kacker *et al.*, *Cryst. Growth Des.* **18**, 312 (2018).

NEW UNDERSTANDING OF COLLECTIVE MODES AND THERMODYNAMICS OF THE LIQUID AND SUPERCRITICAL STATES

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A theory of liquids liquid-glass transition requires understanding most basic thermodynamic properties of the liquid state such as energy and heat capacity. This has turned out to be a long-standing problem in physics [1]. Landau&Lifshitz textbook states that no general formulas can be derived for liquid thermodynamic functions because the interactions are both strong and system-specific. Phrased differently, liquids have no small parameter.

Recent experimental and theoretical results open a new way to understand liquid thermodynamics on the basis of collective modes (phonons) as is done in the solid state theory. There are important differences between phonons in solids and liquids, and we have recently started to understand and quantify this difference. I will review collective modes in liquids including high-frequency solid-like transverse modes and will discuss how a gap in the reciprocal space emerges and develops in their spectrum [2]. This reduces the number of phonons with temperature, consistent with the experimental decrease of constant-volume specific heat with temperature [1]. I will discuss the implication of the above theory for fundamental understanding of liquids. I will also mention how this picture can be extended above the critical point where the recently proposed Frenkel line on the phase diagram separates liquid-like and gas-like states of supercritical dynamics [1,3-5].

[1] K. Trachenko and V.V. Brazhkin, Rep. Prog. Phys. **79**, 016502 (2016).

[2] C. Yang *et al.*, Phys. Rev. Lett. **118**, 215502 (2017).

[3] V.V. Brazhkin and K. Trachenko, Physics Today **65**, 68 (2012).

[4] V.V. Brazhkin *et al.*, Phys. Rev. Lett. **111**, 145901 (2013).

[5] D. Bolmatov *et al.*, Nature Comm. **4**, 2331 (2013).

GLASS TRANSITION IN ULTRASTABLE GLASSES: ANALYZING THE BULK TRANSFORMATION

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Glasses prepared by physical vapour deposition at substrate temperatures around $0.85T_g$ present extraordinary thermodynamic and kinetic stabilities, comparable to those of ordinary glasses aged for thousands of years. Due to their improved packing, these thin film vapour deposited glasses transform into the supercooled liquid via parallel growth fronts that initiate at the free surface/interfaces, at least for the first stages of the transformation [1]. Stability can be further increased by arresting these propagation fronts by capping the surfaces with a higher T_g material [2]. Using this strategy, the glass transition of these ultrastable glasses takes place via a homogeneous transformation mechanism.

In this work we use quasi adiabatic fast-scanning nanocalorimetry to study the characteristics of this homogeneous mechanism in ultrastable glasses. The results show that the kinetic stability during annealing treatments increases by a factor 25–50 with respect to the uncapped stable glasses. In addition, we also identify the existence of two different glass transition mechanisms. Ultrastable glasses transform both via a rejuvenation process that is compatible with a cooperative mechanism, like the one observed in less stable glasses and via a nucleation and growth-like process which dominates the transformation rate.

[1] L.H. Fornander *et al.*, J. Phys. Chem. B **118**, 10795–801 (2015).

[2] F. Rodríguez-Prieto *et al.*, Phys. Chem. Chem. Phys. **20**, 29989–29995 (2018).

COMPLEX LOCAL AND GLASS TRANSITION DYNAMICS IN PA₁₂ STUDIED BY BROADBAND DIELECTRIC SPECTROSCOPY – WHAT CAN WE LEARN FROM HYDRATION EXPERIMENTS?

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In recent years, polyamide 12 (PA 12) has gained specific interest because of its excellent materials and processing properties for selective laser sintering, a 3D printing technique. In particular its moderate melting temperature (180°C), a high crystallization rate along with low shrinkage upon crystallization makes PA 12 a very suitable polymer for this purpose. Like most semi-crystalline polymers, PA 12 forms a morphology consisting of stacked lamellas, however, recent XRD experiments have revealed a rigid amorphous fraction (RAF) that roughly equals the crystalline volume fraction. In this paper we present detailed results from broadband dielectric spectroscopy (BDS) in a wide frequency range (10^{-2} - 10^9 Hz) that show clear dynamic signatures for a three-phase model consisting of a random amorphous, oriented amorphous (RAF) and crystalline fraction. Here, the low-temperature γ -relaxation was assigned to local motions of phase-separated aliphatic chain segments in analogy to the γ -process of LDPE, while the β -relaxation was identified as a PE-like "aliphatic" glass transition process. Both relaxations revealed a fine-structure with selective moisture sensitivity, which support the co-existence of two non-crystalline polymer fractions with different degree of conformational order and hydrogen bonding.

THEORY FOR SWAP ACCELERATION NEAR THE GLASS AND JAMMING

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Swap algorithms can shift the glass transition to lower temperatures, a recent unexplained observation constraining the nature of this phenomenon. Here we show that swap dynamic is governed by an effective potential describing both particle interactions as well as their ability to change size. Requiring its stability is more demanding than for the potential energy alone. This result implies that stable configurations appear at lower energies with swap dynamics, and thus at lower temperatures when the liquid is cooled. The magnitude of this effect is proportional to the width of the radii distribution, and decreases with compression for finite-range purely repulsive interaction potentials. We test these predictions numerically and discuss the implications of these findings for the glass transition. We extend these results to the case of hard spheres where swap is argued to destroy metastable states of the free energy coarse-grained on vibrational time scales. Our analysis unravels the soft elastic modes responsible for the speed up swap induces, and allows us to predict the structure and the vibrational properties of glass configurations reachable with swap. In particular for continuously poly-disperse systems we predict the jamming transition to be dramatically altered, as we confirm numerically. A surprising practical outcome of our analysis is new algorithm that generates ultra-stable glasses by simple descent in an appropriate effective potential.

ORIGIN OF BOSON PEAK IN ORDERED CRYSTALS AND AMORPHOUS SOLIDS

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The vibrational spectra of solids, both ordered and amorphous, in the low-energy regime, control the thermal and transport properties of materials, from heat capacity to heat conduction, electron-phonon couplings, conventional superconductivity etc. The old Debye model of vibrational spectra at low energy gives the vibrational density of states (VDOS) as proportional to the frequency squared, but in many materials the spectrum departs from this law which results in a peak upon normalizing the VDOS by frequency squared, which is known as the "boson peak". A description of the VDOS of solids (both crystals and glasses) is presented. Without using any assumptions whatsoever about the existence and nature of "disorder" in the material, it is shown that the boson peak in the VDOS of both ordered crystals and glasses arises naturally from the competition between elastic mode propagation and viscous damping [1]. The theory explains the recent experimental observations of boson peak in perfectly ordered crystals [2-5], which cannot be explained based on previous theoretical frameworks. The theory also explains, for the first time, how the vibrational spectrum changes with the atomic density of the solid, and explains recent experimental observation [2] of this effect.

[1] M. Baggioli and A. Zaccone, arXiv:1810.09516.

[2] A. I. Chumakov *et al.*, Phys. Rev. Lett. **112**, 025502 (2014).

[3] D. Szewczyk *et al.*, J. Phys. Chem. B **119**, 8468-8474 (2015).

[4] J. F. Gebbia *et al.*, Phys. Rev. Lett. **119**, 215506 (2017).

[5] A. Jezowski *et al.*, Phys. Rev. B **97**, 201201(R) (2018).

EVIDENCE OF A LOW TEMPERATURE DYNAMICAL TRANSITION IN CONCENTRATED MICROGELS

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PNIPAM microgels are nanometer-sized hydrogel particles able to change their behaviour from soft to hard colloids, undergoing a fast and reversible volume phase transition (VPT) from a swollen hydrophilic state to a collapsed hydrophobic state upon increasing temperature. In diluted water solutions, the VPT occurs at about 32°C, increasing with PNIPAM concentrations, making PNIPAM microgels particularly attractive for biomedical applications such as drug delivery. On the other hand, at high concentration PNIPAM microgels are characterized by a complex macromolecular environment which could mimic the multifaceted potential energy landscape of proteins and, in addition, avoid water crystallization allowing the investigation of atomic dynamics at low temperatures. We thus accessed the unexplored high concentration – low temperature region of the PNIPAM phase diagram, studying PNIPAM ps atomic dynamics by means of elastic incoherent neutron scattering (EINS) and all atom molecular dynamics (MD) simulations. We observe the occurrence of a "dynamical transition" at about 250 K, similar to that observed in proteins. The transition temperature does not show a dependence on PNIPAM mass fraction, but the transition tends to disappear on approaching dry conditions. The quantitative agreement between experiments and simulations provides evidence that the transition occurs simultaneously for PNIPAM and water dynamics. The similarity of these results with hydrated protein powders suggests that the dynamical transition is a generic feature in complex macromolecular systems, independently from their biological function.

[1] M. Zanatta *et al.*, *Sci. Adv.* **4**, eaat5895 (2018).

[2] L. Tavagnacco *et al.*, *J. Phys. Chem. Lett.* **10**, 870-876 (1019).

SHORT-TIME DYNAMICS OF CONFINED COLLOIDS PROBED BY HIGH-ENERGY COHERENT X-RAYS

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Dense colloidal suspensions show a complex wave-vector dependent dynamics, depending on particle-particle interactions that can be direct (e.g. hard, soft-sphere like) and indirect through the hydrodynamic interaction mediated by the solvent [1,2]. In bulk the diffusion behavior is generally isotropic but in confined geometry anisotropic dependences emerge as soon as particles are confined between two walls spaced by few particles diameters [3]. Here we apply X-ray Photon Correlation Spectroscopy (XPCS) in small-angle scattering geometry to study a colloidal suspension confined between channels of a microfluidic device [4]. We show that the hydrodynamic function in the short-time limit is strongly anisotropic similarly to what is observed for the structure factor [5].

The work highlights the application of coherent high-energy X-rays, a key feature of the upcoming Extremely Brilliant Source at ESRF. The promised 100 fold increase in brilliance will expand the use of XPCS up to 35 keV, opening the door to systems implying bulky environments, e.g. diamond anvil cell for high-pressure research, and easing the study of radiation sensitive materials like soft and biological systems.

[1] V.A. Martínez *et al.*, J. Chem. Phys. **134**, 054505 (2011).

[2] A.J. Banchio *et al.*, Phys. Rev. Lett. **96**, 138303 (2006).

[3] K. Nygård *et al.*, Phys. Rev. Lett. **108**, 037802 (2012).

[4] K. Nygård *et al.*, Phys. Rev. Lett. **116**, 167801 (2016).

[5] K. Nygård *et al.*, Phys. Rev. E **95**, 062601 (2017).

Part III

Posters

THE EXP PAIR-POTENTIAL SYSTEM

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It was recently shown that the exponentially repulsive EXP pair potential defines a system of particles in terms of which simple liquids' quasiuniversality may be explained [1,2]. The quasiuniversality was illustrated by showing that the structure of the Lennard-Jones system at four state points is well approximated by those of EXP pair-potential systems with the same reduced diffusion constant [3].

The fluid phase of the EXP pair potential system was studied in two companion papers [3,4]. The study revealed the existence of two regions in the fluid: A gas phase and a liquid phase which are distinguished pragmatically by the absence or presence of a minimum in the radial distribution function above its first maximum. The existence of isomorphs has been found in both the dilute gas phase, and in the condensed liquid. The simplicity of the gas phase allows for predictions of the virial potential-energy Pearson correlation coefficient R and the density-scaling exponent in the dilute limit.

In the latest work also the crystal phase has been studied and both a bcc phase and a fcc phase has been found (unpublished).

- [1] A.K. Bacher *et al.*, Nat. Comm. **5**, 5424 (2014).
- [2] J.C. Dyre, J. Phys. Condens. Matter **28**, 323001 (2016).
- [3] A.K. Bacher *et al.*, J. Chem. Phys. **149**, 114501 (2018).
- [4] A.K. Bacher *et al.*, J. Chem. Phys. **149**, 114502 (2018).

EFFECT OF OPTICAL PHONONS ON THE VIBRATIONAL SPECTRUM AND ON THE LOW-T SPECIFIC HEAT OF SOLIDS

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It has been shown that the so-called THz anomalies observed in solids (both crystals and glasses), and known as the boson peak (BP), universally appear from the competition between viscous damping and elastic propagation of the acoustic phonons. The effect of the optical phonons on the vibrational spectrum of solids, instead, has received very little attention and a theory of vibrational spectra of solids including optical modes is missing. Recent experimental results have pointed at the importance of optical modes in the low-energy vibrational spectrum of solids, including both covalently bonded and molecular crystals. Here we study the contribution of optical modes to the vibrational density of states and to the specific heat. We prove that light, or weakly gapped, optical modes contribute to the BP and most importantly they provide a contribution to the density of states and the specific heat analogous to the two-level systems in glasses. Clearly in a crystal there are not two level systems, therefore the emerging scenario is that the experimental observation of such anomalies in ordered crystals can be due to the presence of low-energy optical modes which thus explains recent experimental observations.

EFFECT OF OPTICAL PHONONS ON THE VIBRATIONAL SPECTRUM AND ON THE LOW-T SPECIFIC HEAT OF SOLIDS

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Ionic liquids (ILs) are salt in liquid state that are characterized by low melting point and vapour pressure, good thermal stability and high ionic conductivity. Thanks to these properties, ILs are a promising class of technologically useful and interesting materials. Water represents an excellent partner for ILs because it exhibits a wide variety of peculiar properties that can be complementary to those possessed by pure ILs, such as the capacity to hydrate biomolecules and to form extended hydrogen-bond networks. For example, it has been recently suggested that the conformational stability of Deoxyribonucleic acid (DNA) can be significantly improved in ILs-water mixture with respect the solvation in pure water. UV Resonant Raman (UVR) scattering can provide insights on the structural rearrangements and conformational changes in IL-water mixtures at different experimental conditions, through the measurement of the molecular vibrations of the system. Both selectivity and sensitivity of the technique can be improved by the resonance effect, which enhance specific vibrational signals of targeted molecular groups, through an appropriate tuning of the excitation wavelength. In this talk, we will present some results that illustrate the ability of UVR spectroscopy to investigate, at molecular level, the solvation properties of different ILs-water mixtures, also in the presence of biological macromolecules as DNA, with selectivity on specific portions of the system.

ESHELBY DESCRIPTION OF HIGHLY VISCOUS FLOW

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The highly viscous flow is due to thermally activated Eshelby transitions which transform a region of the undercooled liquid to a different structure with a different elastic misfit to the viscoelastic surroundings. A self-consistent determination of the viscosity in this picture explains why the average structural relaxation time is a factor of eight longer than the Maxwell time. The physical reason for the short Maxwell time is the very large contribution of strongly strained inherent states to the fluidity (the inverse viscosity). At the Maxwell time, the viscous no-return processes coexist with the back-and-forth jumping retardation processes [1].

[1] U. Buchenau, J. Chem. Phys. **148**, 064502 (2018).

[2] U. Buchenau, J. Chem. Phys. **149**, 044508 (2018).

MULTISCALE MODELLING AND SCALING THEORIES FOR POLYMER BRUSHES

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Polymer brushes are complex macromolecular assemblies able to perform the most diversified tasks.

We will explore properties of polymeric brushes of different geometries and chemical compositions. Starting from simple scaling theories up to more complex multiscale methodologies, we will show how to characterise the properties of the various systems, and how to exploit such materials to perform simple work.

The role of geometry in a controlled and tunable adsorption process or the role of chemical composition in designing a controlled patterning on a substrate will be predicted by means of theoretical previsions and explored by means of computational methods relying on a controlled approach. Finally we will show how to experimentally realize such functionalized systems

MICRO-EV VIBRATIONAL DYNAMICS IN AMORPHOUS SiO_2

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Glasses at low temperature (below 10 K) are characterized by thermal and vibrational properties that are markedly different from those of crystals [1]. In particular, long-wavelength phonons are considerably more damped in glasses, which is often explained in terms of Rayleigh scattering of sound waves by local elastic heterogeneities uncorrelated in space. Experimental results have been claimed to agree with this scenario, that predicts phonon damping to increase with the fourth power of phonon energy [2,3].

This interpretation has been recently questioned, and in particular it has been argued that a logarithmic correction to the dominant Rayleigh scattering term appears both in simulations and in experimental data and is the signature of long-range spatial correlations of elastic disorder [4]. This is claimed to be a crucial feature that distinguishes amorphous solids from crystals. A way to test this newly proposed scenario is to measure the low-frequency tail of the vibrational density of states (DOS). This tail, whose frequency dependence is directly related to phonon damping [5], can indeed provide direct information of the existence of long-range elastic correlations in glasses. However, very high energy resolution (<1 meV) and high enough fluxes are required. The combination of the new spectrograph implemented at the ID18 beamline of the ESRF with nuclear resonance analysis of inelastic scattering (NRAIXS) [6] technique allowed us to overcome these limitations and measure the density of state of the prototypical glass former SiO_2 well below 1 meV.

Here the experimental scheme will be described in detail and the preliminary results on SiO_2 will be presented.

[1] R.C. Zeller and R.O. Pohl, *Phys. Rev. B* **4**, 2029 (1971).

[2] G. Monaco and V. Giordano, *PNAS* **106**, 3659 (2009).

[3] G. Baldi *et al.*, *Phys. Rev. Lett.* **104**, 195501 (2010).

[4] S. Gelin *et al.*, *Nat. Materials* **15**, 1177 (2016).

[5] W. Schirmacher *et al.*, *Phys. Rev. Lett.* **98**, 025501 (2007).

[6] A.I. Chumakov *et al.*, *Phys. Rev. Lett.* **76**, 4258 (1996).

ENHANCING THE MOLECULAR COOPERATIVITY OF POLYVINYL BUTYRAL USING LIQUID ADDITIVES

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The specific role of acetonitrile and methoxypropionitrile, as accelerators of the relaxation dynamics of polyvinyl butyral (PVB), was investigated in polymer/additive mixtures with a saturation liquid content. The aim was to improve the ionic mobility of PVB-based solid electrolytes to be used in solid dye-sensitized solar cells. Mechanical and dielectric relaxation measurements between 120 K and 380 K revealed that the β -relaxation observed above 330 K in dry-PVB is shifted quite below room temperature in PVB/additives. Both the additives cause a growing intermolecular cooperativity, the sub-glass β -relaxation exhibiting a strength enhanced by a factor 3 and a frequency factor which increases from 10^{15} s^{-1} up to 10^{21} s^{-1} . This discloses an activation entropy as high as 165.7 J/K mol in comparison to 40.8 J/K mol in dry-PVB. It is suggested the existence of cooperative transitions, mainly driven by bridges formed through additive molecules, which influence both short- and long-scale segmental motions and also favor the ion dynamics in PVB/additive/electrolyte systems. The room temperature ionic conductivity σ_{rt} exhibits large changes from $6.4 \cdot 10^{-14} \text{ S/m}$ in dry PVB, through $1.5 \cdot 10^{-8} \text{ S/m}$ in PVB/LiI, to $2.45 \cdot 10^{-5} \text{ S/m}$ in PVB/MPN/LiI.

HYDRATION OF THE TRIPEPTIDE GLUTATHIONE PROBED BY UV RAMAN SPECTROSCOPY

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A better understanding of the interactions and dynamics that exist between the solvent and the biological macromolecules, such as proteins and peptides, is the key to knowing how these macromolecules are able to perform their functions within the human body. In particular, the biological activity of peptides is strictly connect to the solvent properties that plays a fundamental role in driving the function of these molecules. A description, at the atomic scale, of water solvation can provide insights on still open and important issues, like protein folding and association as well as protein-ligand binding processes. For a better comprehension of this subject, we decided to investigate the interaction between water and specific groups of the tripeptide Glutathione. The choice of Glutathione as case study, it has been suggested because this molecule presents a simpler structure compared with that of the proteins, therefore, the rationalization of the tripeptide behaviour, in function of the different parameters, will be easier. Moreover, Glutathione is an important constituent of the living systems that protect cells components against oxidation. In this work, has been investigated by UV Resonant Raman Spectroscopy the solvent dynamics around specific sites of Glutathione, as probed by the spectral changes observed as a function of pH, peptide concentration and temperature.

GENERAL METHODOLOGY TO IDENTIFY THE MINIMUM ALPHABET SIZE FOR HETEROPOLYMER DESIGN

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Understanding how to design the structure of heteropolymers through their monomer sequence will have a significant impact on the creation of novel artificial materials. According to mean field theories, the minimum number – or alphabet– of distinct monomers necessary to achieve such designability is directly related to the conformational entropy ω of compact polymer structures. Here we introduce a computational strategy to calculate this conformational entropy and thus predict the minimum alphabet to achieve designability, for a generalised heteropolymer model. The comparison of our predictions with previous results proves the robustness of our approach. We quantify for the first time how the number of directional interactions is critical for achieving the designability. The methodology we introduce can be easily generalised to models representing specific polymers. We provide a comparison between conventional polymers monomers, and we predict that polyurea, polyamide and polyurethane residues are optimal candidates to be functionalised for the experimental synthesis of designable heteropolymers. As such, our method can guide the engineering of new types of self-assembling modular polymers, that will open new possibilities for polymer-based materials with unmatched versatility and control.

DESIGNING AN OPTIMAL ION ADSORBER AT THE NANOSCALE: THE UNUSUAL NUCLEATION OF AgNPs/Co²⁺-Ni²⁺ BINARY MIXTURES

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Selective removal of heavy metals from water is a complex topic. We present a hybrid experimental/theoretical-computational approach to design a functionalised nanomaterial able to selectively capture metallic ions from water within a self-assembling process. A theoretical model is used to map an experimental mixture of Ag nanoparticles (AgNPs) and either Co²⁺ or Ni²⁺ onto an additive highly asymmetric attractive Lennard-Jones binary mixture. Extensive NVT Monte Carlo simulations are performed to deduce the set of parameters that first induce aggregation amongst the two species in solution, and then affect the shape of the aggregates. The computational predictions are thus compared to the experimental results. The gathered insights can be used as guidelines for the prediction of an optimal design of a new generation of selective nanoparticles to be used for metallic ion adsorption hence for maximising the trapping of ions in an aqueous solution.

REVISITING THE STOKES-EINSTEIN RELATION WITHOUT A HYDRODYNAMIC DIAMETER

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We present diffusion coefficient and shear viscosity data for the Lennard-Jones fluid along nine isochores above the critical density, each involving a temperature variation of roughly two orders of magnitude. The data are analyzed with respect to the Stokes-Einstein (SE) relation, which exhibits a gradual breakdown at high temperatures. This is rationalized in terms of the fact that the reduced diffusion coefficient \tilde{D} and the reduced viscosity $\tilde{\eta}$ are both constant along the system's isomorphs [1]. It is shown that $\tilde{D}\tilde{\eta}$ is a function of $T/T_{Rel(\rho)}$ in which T is temperature, ρ is density, and $T_{Rel(\rho)}$ is the temperature along a reference isomorph. This allows one to successfully predict the viscosity from the diffusion coefficient throughout the studied region of the thermodynamic phase diagram, also for the state points at which SE does not apply [3]. The viscosities calculated in this way are found to be in good agreement with the equation previously proposed in Ref. [2].

[1] N. Gnan *et al.*, J. Chem. Phys. **131**, 234504, (2009).

[2] L. Costigliola *et al.*, J. Chem. Phys. **148**, 081101, (2018).

[3] Submitted to J. Chem. Phys.

RELATION BETWEEN FRACTAL DIMENSION AND TOPOLOGICAL INVARIANTS TO EVALUATE COMPLEXITY IN ABSTRACT IMAGES

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Felix Hausdorff helps Mandelbrot to win the sky giving to him the wings with the mathematical description of the fractals. Even though, for topologist the definition is incomplete. The measure of complexity in complex patterns has been a method to describe the intrinsic dynamics in physical phenomena. The evaluation of physical structures by fractality and Betti numbers has been widely studied; nevertheless, there remains a need for distinguish the information obtained by these parameters. This work focus on describing the relation between structural properties measured by Fractal dimension and complexity evaluated by topological invariants measured by Betti numbers. By considering two dimensional abstract images constructed by points and lines, we compare the information obtained by these two parameters. Investigations in which complex structures of art are studied objectively are scarce. Our study may inspire multidisciplinary investigators to consider mathematical tools to evaluate other complex structures.

MULTI-COMPONENT GLASSES AND THEIR SUITABILITY FOR NUCLEAR WASTE ENCAPSULATION

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Multi-component glasses have long been used for encapsulating nuclear waste [1], but an understanding of the glass's stability over geological time scales and the effects of radiation damage is required. Experiment shows that stored energy in waste glasses increases with α -particle dose, associated with an increase in defects, but that observed volume changes are most likely due to a rearrangement of the glass network as a result of the α -recoil nuclei [2]. Though radiation damage effects have been simulated in crystalline materials, to our knowledge borosilicate glasses have only been simulated with low recoil energies (< 1 keV) [3], meaning higher energy recoils must be studied to determine the nature of defects and network rearrangement. Higher energy radiation damage simulations require amorphous systems of 10s of millions of atoms, requiring the development of on the fly analysis tools for DL-POLY [4] for tracking the formation of defects, which are harder to identify in amorphous systems. We will present the structural and material properties of multi-component glasses determined from MD simulations, and the underlying atomistic picture of defect generation and glass network rearrangement due to radiation damage.

[1] I.W. Donald *et al.*, *J. Mater. Sci.* **32**, 5851-5887 (1997).

[2] W.K. Weber, *Proc. Mat. Sci.* **7**, 237-46 (2014).

[3] D.A. Kilymis *et al.*, *J. Non-Cryst. Solids* **432**, 354-360 (2016).

[4] I.T. Todorov *et al.*, *J. Mater. Chem.* **16**, 1911-8 (2006).

TREHALOSE PROTECTANT ACTIVITY FOR PEPTIDE HYDRATION

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The interactions of carbohydrates with biomolecules are of great interest, as these interactions are responsible for their protection against environmental stresses. Among the different bioprotectants, the disaccharide trehalose is the best performer. To date there are three possible hypotheses that try to explain structural and dynamical mechanisms of bioprotective features. The first is the substitution, in which the trehalose replaces the water molecules of the first hydration shell, maintaining peptide structure and functionality [1]. The second is the vitrification, where trehalose interacts with water and the system undergoes a glass-like stabilizing transition [2]. The third is the confinement, where a few water molecules mediate the peptide-sugar interaction and trehalose creates a cage around the hydrated molecules [3]. To clarify which of these hypotheses better describes the real situation, a series of neutron diffraction with H/D isotopic substitution experiments, combined with EPSR computer simulations, have been performed. The results highlight that the addition of trehalose in solution does not alter the peptide first hydration shell and that trehalose forms a protective cage around the hydrated peptide. Therefore, this data don't sustain the substitution hypothesis.

[1] J.H. Crowe *et al.*, *Science* **223**, 701-703 (1984).

[2] J.L. Green *et al.*, *J. Phys. Chem.* **93**, 2880-2882 (1989).

[3] R.D. Lins *et al.*, *Proteins* **55**, 177-186 (2004).

HIDDEN SCALE INVARIANCE IN LIQUID CuZr

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Metallic systems are a very important category of glass former due to their possible applications in material science as well as their suitability as a model system to study the glass transformation in simulations. It has recently been discovered that materials with non-directional bonding (like metals) exhibit a particular (Roskilde) simple behaviour due to an underlying hidden scale invariance as described in isomorph theory [1, 2]. Isomorphs (identified as configurational adiabats) are curves in the phase diagrams along which structure and dynamics are predicted to be invariant (in appropriately reduced units) to a good approximation.

This work studies different compositions of the well known binary glass-former $\text{Cu}_x\text{Zr}_{100-x}$ ($x = 36, 50, 64$) in the context of isomorph theory, investigating structure and dynamics by means of the radial distribution function, the intermediate scattering function and the mean-squared displacement. In order to model the metals realistically, the atomic interactions are simulated using effective medium theory [3], a many-body potential similar to the embedded atom method.

We present results for the invariance of structure and dynamics and find good collapse up to density changes of well over 50%. All simulations are carried out using the Roskilde University Molecular Dynamics (RUMD) software package.

[1] L. Böhling *et al.*, *New J. Phys.* **14**, 113035 (2012).

[2] F. Hummel *et al.*, *Phys. Rev. B* **92**, 174116 (2015).

[3] K.W. Jacobsen *et al.*, *Surf. Sci.* **366**, 394 (1996).

A COMPACT DEVICE FOR SIMULTANEOUS DIELECTRIC SPECTROSCOPY AND GRAVIMETRIC ANALYSIS USING QUARTZ CRYSTAL MICROBALANCE UNDER CONTROLLED HUMIDITY

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Hydration of natural or synthetic macromolecules is responsible for a variety of phenomena, affecting both the structure and the stability of such systems. Measuring the effect of hydration enhances the understanding of many complex biological mechanisms such as protein folding [1-2], as well as the dynamics and conformations of polymers [3-4].

Simultaneous quantification of the film thickness while monitoring the evolution of the dynamics upon thickness variation would be a great advantage. In this study, a newly designed cell has been presented, which allows setting a standardized humidity and in parallel measuring the mass loss/uptake using a quartz crystal balance (QCM). This setup has been successfully fabricated and validated at different conditions. Moreover, we performed dielectric measurements on DMPC multilamellar vesicles (MLV) to examine the interplay between the hydration water and lipid multilayer in a frequency region from 0.1 Hz up to 1 MHz.

It was shown that at low hydration levels more pronounced lipids phase transitions are revealed and how humidity affects the T-dependence of the main lipid phase transition. The data acquired by dielectric spectroscopy were supported by *in situ* mass loss and uptake as revealed by QCM results.

[1] M. Yang *et al.*, *Polymer Phys.* **55**, 1859-1864 (2017).

[2] J.L. MacCallum *et al.*, *PNAS* **112**, 6985-6990 (2015).

[3] F. Khabaz *et al.*, *Macromolecules* **49**, 7551-7562 (2016).

[4] G. Paradossi *et al.*, *Polymers* **3**, 1805-1832 (2011).

MOLECULAR DYNAMICS OF BINARY MIXTURES OF IBUPROFEN WITH OCTAACETYLMALTOSE NEAR THE GLASS TRANSITION

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Many crystalline drugs are poorly water-soluble and their bioavailability is limited. A very promising way to improve the water solubility of medicines is their transformation to the amorphous form. However, amorphous pharmaceuticals tend to recrystallize. The preparation of amorphous binary mixtures of a drug with some excipients is currently considered as an effective method for enhancing the physical stability of amorphous drugs [1,2]. In this work, we study the effect of gradual adding octaacetylmaltose (acMAL) to ibuprofen (IBU) on the molecular dynamics and the physical stability of the drug in the binary mixtures by means of the broadband dielectric spectroscopy and temperature modulated differential scanning calorimetry. These binary systems are interesting because IBU molecules can form H-bonds with IBU (IBU \cdots IBU) and acMAL molecules (IBU \cdots acMAL), while acMAL molecules cannot form H-bonds between themselves (only van der Waals interactions). By changing the content of acMAL in the mixture (IBU+acMAL), we also modify the character of intermolecular interactions in investigated systems. We study how molecular dynamics factors (i.e., glass transition temperature, fragility, dynamic heterogeneity) reflect the changes in the nature of intermolecular interactions related to the different content of acMAL in the binary mixtures.

[1] K. Grzybowska *et al.*, *Adv. Drug Deliv. Rev.* **100**, 158 (2016).

[2] K. Grzybowska *et al.*, *Mol. Pharmaceutics* **14**, 1154 (2017).

MATHEMATICAL MODELING OF POLYMERIC MATERIALS: FINSLER GEOMETRY MODELS AND MONTE CARLO SIMULATIONS

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Polymeric materials such as liquid crystal elastomer (LCE) and rubbers, etc. are interesting because of their non-standard mechanical properties. Indeed, the stress-strain diagram of LCE has a plateau, which is called soft elasticity, and the strain of rubbers is very large; up to 500% or more. For the proper understanding of these elasticities, a considerable number of studies have been conducted. In this talk, we present the results obtained by Finsler geometry (FG) modeling and Monte Carlo simulations for polymeric materials such as LCE [1-3], two-components artificial membrane [4,5], soft-biological materials [6,7], and rubbers [8], and we show that the FG modeling is effective for studying such complex phenomena. It will also be presented why FG modeling is interesting and effective as a study tool for these materials. This work is supported in part by JSPS KAKENHI Grant Number JP17K05149 and the Collaborative Research Project of the Institute of Fluid Science, Tohoku University.

- [1] K. Osari and H. Koibuchi, *Polymer* **114** 355-369 (2017).
- [2] E. Proutorov *et al.*, *J. Phys. (Cond. Matt.)* **30**, 405101 (2018).
- [3] H. Koibuchi, *Polymers* **10**, 757 (2018).
- [4] S. Usui and H. Koibuchi, *Polymers* **8**, 284 (2016).
- [5] E. Proutorov and H. Koibuchi, *Axioms* **6**, 10 (2017).
- [6] Y. Takano and H. Koibuchi, *Phys Rev. E* **95**, 042411 (2017).
- [7] K. Mitsuhashi *et al.*, *Polymers* **10**, 715 (2018).
- [8] H. Koibuchi *et al.*, in preparation.

EVOLUTION OF PROPERTIES OF THIN FILM MIXTURES OF HYDROGEN-BONDED MOLECULES AT LOW TEMPERATURES

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The processes of deposition, sublimation and secondary deposition of gases at low temperatures are an integral part of the heat-mass transfer phenomena in cryogenic-vacuum equipment and are of high relevance for operation of optical devices in space conditions. It is well-known that the considerable amount of substance in the Universe represents multi-component ices cryogenically deposited on the surface of space objects. Under the influence of external factors, such ices may undergo phase transitions, wherein some of their components may evaporate, leading to structural transformation of the remaining material. Consequently, a new phase is formed, whose properties depend on cluster composition of the remaining material as well as the surface temperature. Such processes may be modeled using cryogenic equipment in a laboratory environment. The current work is aimed at a comprehensive study of formation, evolution and restructuring of thin film mixtures of ethanol and methanol with an inert argon host material, following evaporation of the latter. The samples are formed during cryovacuum deposition of the test substance from the gas phase to the substrate at low temperatures in the range from 10 K to 40 K and gas pressures from 10^7 Torr to 10^3 Torr. The thickness of the sample varies from 10 μm to 100 μm .

RUMD: A GENERAL PURPOSE MOLECULAR DYNAMICS PACKAGE OPTIMIZED TO UTILIZE GPU HARDWARE DOWN TO A FEW THOUSAND PARTICLES

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RUMD is a general purpose, high-performance molecular dynamics (MD) simulation package running on graphical processing units (GPU's). RUMD addresses the challenge of utilizing the many-core nature of modern GPU hardware when simulating small to medium system sizes (roughly from a few thousand up to hundred thousand particles). It has a performance that is comparable to other GPU-MD codes at large system sizes and substantially better at smaller sizes. RUMD is open-source and consists of a library written in C++ and the CUDA extension to C, an easy-to-use Python interface, and a set of tools for set-up and post-simulation data analysis. The paper describes RUMD's main features, optimizations and performance benchmarks [1].

[1] N.P. Bailey *et al.*, *SciPost Phys.* 3, 038 (2017).

THE SUPERCOOLED LIQUID STATE OF GLASS-FORMING LIQUIDS

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Nowdays, despite the intense research in the topic, does not exist any first-principles theory which provides a satisfactory understanding of the glass transition and physical aging. In the present work, the recently developed, Non-Equilibrium Self-Consistent Generalized Langeving Equation (NESCGL) theory is used to predict the final state of glass-forming liquids subjected to different cooling processes. We show that the NESCGL describes the principal features which characterize the glass transition. Such features are, the structural recovery (the tendency of the overall microscopic structure towards its equilibrium value), the universality of the glass transition temperature, the dependence of the final state with the cooling rate, among others. We demonstrate that only for a quasi-static process the equilibrium line could be reached. The qualitative comparisons with the observed phenomenology, such the enthalpy recovery plateau, shows the reliability of the NESCGL as a definitive theory for the glass transition.

FOLLOWING THE BEHAVIOR OF THE LINEAR VISCOELASTICITY ON ARRESTED SPINODAL DECOMPOSITION

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The recent non-equilibrium self-consistent generalized Langevin equation (NE-SCGLE) theory of irreversible process in liquids [1,2] has permitted to obtain a description of non-equilibrium processes involved in the arrested spinodal decomposition due to sudden and deep quenches inside the spinodal region. For a simple model liquid, where the system could be modeled by a hard sphere plus an attractive Yukawa tail, this theoretical approach predicts that the spinodal line is the borderline between the ergodic and the arrested states. Also, using this approach has been determined a border between phase separation and gelation, besides providing the corresponding dynamic properties to each phase [3]. This work addresses a general method to obtain the linear viscoelastic properties of non-equilibrium processes involved in the spinodal decomposition when the system has been quenching inside the spinodal region. In Fig. (1), we show an example of the normalized shear viscosity as a function of the waiting time. This scheme offers the opportunity to describe the linear viscoelasticity and the diffusion mechanics as the waiting time elapses. Furthermore, this approach can describe gelation effects, and it leads naturally to a diverging shear viscosity at glass and gelation transition points.

[1] P.E. Ramírez-González and M. Medina-Noyola, *Phys. Rev. E* **82**, 061503 (2010).

[2] P.E. Ramírez-González and M. Medina-Noyola, *Phys. Rev. E* **82**, 061504 (2010).

[3] J.M. Olais-Govea *et al.*, *J. Chem. Phys.* **143**, 174505 (2015).

ESTIMATION OF EFFECTIVE BRAIN CONNECTIVITY USING A RECURRENT NEURAL NETWORK MODEL ON MAGNETOENCEPHALOGRAPHY DATA

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The functional communication mechanism within the brain is given by synchronous neural activity among its different regions. Electroencephalography (EEG) and Magnetoencephalography (MEG) are among the most prominent tools to study noninvasively and with high temporal resolution brain synchronization phenomena. Brain connectivity, in particular, can be subdivided into three types: neuroanatomical (or structural), functional (measured performing cross-correlation) and effective connectivity (referred to a pattern of causal interactions between distinct units within a nervous system). The analysis on these different levels is crucial to elucidate how the units of brain process information through the relationship that links together these three different brain connectivity definitions and it represents a significant challenge in the field of neuroscience. Here, we present a new computational protocol which is able to determine the connectivity matrix starting from MEG data. The evolution of the signal over time has been used to infer the matrix of causal connections through the use of a recurrent neural network model and the Backpropagation Through Time method, where the neural networks are networks formed by binary McCulloch-Pitts neurons. The basic idea is that if we are able to learn from the transitions of brain states over time, then we can determine causal relationships among brain units and predict future brain states starting from a specific brain configuration.

AN EXPLORATION–EXPLOITATION TRADEOFF DICTATES THE OPTIMAL DISTRIBUTION OF PHENOTYPES FOR POPULATIONS IN PRESENCE OF FITNESS FLUCTUATIONS

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We study a minimal model for the growth of a phenotypically heterogeneous population of cells subject to a fluctuating environment in which they can replicate (by exploiting available resources) and modify their phenotype within a given landscape (thereby exploring novel configurations). The model displays an exploration–exploitation trade-off whose specifics depend on the statistics of the environment. Most notably, the phenotypic distribution corresponding to maximum population fitness (i.e. growth rate) requires a non-zero exploration rate when the magnitude of environmental fluctuations changes randomly over time, while a purely exploitative strategy turns out to be optimal in two-state environments, independently of the statistics of switching times. We obtain analytical insight into the limiting cases of very fast and very slow exploration rates by directly linking population growth to the features of the environment.

LOW-TEMPERATURE SPECIFIC HEAT OF GLASSES AND DISORDERED SOLIDS

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The physical properties at low temperatures in crystalline and amorphous solids are clearly different. For the heat capacity case, the crystal presents a cubic dependence with temperature (Debye theory), whereas in the amorphous or glassy state a linear-term contribution dominates below 1 K, which is associated to the existence of tunneling two-level systems (TTLs). Above 1 K, there are still other contributions to the specific heat in excess to the one foreseen by the Debye theory, which produce a broad maximum in the Debye-reduced specific heat C_p/T^3 . In the last decades, another group of materials obtained by quenching plastic crystal phases, named glassy crystals, presents a glassy behavior whereas they have positional order, but orientational disorder.

In this work, we present specific heat data of different kinds of disordered solids, measured above 1.8 K.

On the one hand, the halomethanes system $\text{CCl}_{4-n}\text{Br}_n$ ($n = 0, 1, 2$) presents a stable crystalline phase at low temperatures. However, the existence of an *occupational* disorder ($n \neq 0$) of the different halogen atoms in the crystalline lattice appears to produce a clear glassy behavior in the specific heat. Surprisingly, also CCl_4 shows glassy behavior [1].

On the other the hand, for the toluene case both crystalline and glassy states can be achieved, though 2% mol of ethanol doping for avoiding crystallization. In its crystalline phase, toluene exhibits the usual crystalline behavior. Nevertheless, in the glassy state toluene does not show the full glassy behavior since TTLs are absent within our experimental error [2].

[1] M. Moratalla *et al.*, submitted.

[2] M. Moratalla *et al.*, *Low Temp. Phys.*, accepted

CAN ONE AFFORD TO OVERLOOK THE FUNDAMENTAL ROLE OF THE JG β -RELAXATION?

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Experimental evidences in conjunction with the Coupling Model were used in 1998 to suggest the universal presence of secondary relaxation having properties strongly connected to the primary α -relaxation [1]. We called these secondary relaxations the Johari-Goldstein β -relaxation in order to distinguish them from other secondary relaxations without any connection. This remarkable finding is amply supported by the discovery in the last twenty years of more connections in properties between the JG β -relaxation and the α -relaxation. Examples include the following.

(a) The JG β -relaxation time τ_β at T_g of many molecular and polymeric glass-formers correlates with the width of the frequency dispersion of the α -relaxation with $n = (1 - \beta_k)$ where β_k is fractional exponent of the Kohlrausch α -correlation function.

(b) The JG β -relaxation like the α -relaxation is sensitive to applied pressure P and the ratio τ_β/τ_α of their relaxation times is invariant to wide variations of P and T while keeping τ_α constant.

(c) Both τ_α and τ_β are functions of the *same* thermodynamic scaling variable, $T\rho^{-\gamma}$, where ρ is the density and γ is a material constant. Since the JG β -relaxation is the precursor of the α -relaxation, this implies that the $T\rho^{-\gamma}$ -dependence of τ_α originates from τ_{JG} .

(d) Caged dynamics (as observed at high frequencies in the glassy state by THz spectroscopy, neutron scattering NMR, etc.) changes its T -dependence at the JG β glass transition temperatures $T_{g\beta}$ as well as at $T_{g\alpha}$.

(e) The analogue of the JG β -relaxation is found in ionic liquids as the conductivity β -relaxation, and the conductivity β -relaxation time has the same relation to the conductivity α -relaxation as properties (a)-(d).

These examples of the strong connection between the JG β -relaxation to the α -relaxation and the caged dynamics indicate its fundamental importance and should not be overlooked in attempts to fully understand the dynamics.

[1] K.L. Ngai, J.Chem.Phys. **109**, 6982 (1998).

[2] K.L. Ngai and M. Paluch, J.Chem.Phys. **120**, 857 (2004).

[3] S. Valenti *et al.*, J.Chem.Phys. **148**, 054504 (2018)

FEL APPROACH TO AGING PHENOMENA

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The free energy landscape theory is a versatile approach to non-equilibrium systems and has provided a theoretical frame work for unified understanding of glass transition and related singular behaviors [1].

In this presentation, I discuss the aging phenomena on the basis of the FEL approach. I first consider the dielectric relaxation represented by a simple two-level system and discuss the waiting time, t_w , dependence of the polarization and the linear susceptibility when the temperature is suddenly changed at time $t = 0$. I assume that the transition rate relaxes with relaxation time τ_F and show that the relaxation of the FEL manifests itself in the aging effect, namely in an extra t_w dependence of observables on top of the simple term depending on $t - t_w$.

Next, I consider the dynamics of an order parameter given by Lagrangian $\mathcal{L}(M, \dot{M}) = \dot{M}^2/2 - \Phi(M, T)$ and a dissipation term $\mathcal{F}(\dot{M}) = k\dot{M}^2/2$, where $A(T)$ in the Landau free energy $\Phi(M, T) = \Phi_0 + A(T)M^2 + BM^4 - HM$ is assumed to have a delayed response to the temperature modulation with relaxation time τ_F . When the temperature is modulated sinusoidally, I show that there appear second order responses at the sum and the difference of the frequencies of the external field and the temperature modulation and that the relaxation time of the FEL can be deduced from the ratio of these two responses.

[1] T. Odagaki, J. Phys. Soc. Jpn. **86**, 082001 (2017).

LATENT ARRESTED SPINODAL DECOMPOSITION AND INTERFERENCE BETWEEN THE GLASS, GEL, AND GAS-LIQUID TRANSITIONS

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The kinetic perspective of the non-equilibrium self-consistent generalized Langevin equation (NESCGL) theory of irreversible processes in liquids is applied here to study the interference between the non-equilibrium glass and gel transitions, and the gas-liquid equilibrium phase transition, of "Lennard-Jones-like" liquids instantaneously quenched to a final temperature T_f below the spinodal temperature T_s . The results reveal an unexpectedly rich and complex kinetic scenario, that describes spinodal decomposition, gelation, glass transition, and their combinations, within a common first-principles microscopic theoretical framework. For shallow quenches a dominant role is played by a "latency" time t_l characterizing an initial pseudo-equilibration stage, in which the system remains fluid and the dynamic arrest stays latent. This latency time $t_l(T_f)$ depends on T_f and is predicted to diverge as T_f approaches T_s from below. For deeper quenches $t_l(T_f)$ decreases to microscopic dimensions, and the dynamics exhibits a three-step relaxation associated with a predicted low-temperature gel-glass transition.

THE NON-DEBYE SPECTRUM IN STRUCTURAL GLASSES AND SUPERCOOLED LIQUIDS

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At small enough frequencies glasses and disordered solids follow Debye's law. This is because at large length scales they are continuum media and thus phonons, i.e., Goldstone bosons, dominate the low frequency spectrum. However, the mechanical and thermodynamic properties of glasses, even though universal, deviate from those in crystalline solids. These anomalies imply peculiar and universal deviations from Debye's law at low frequencies. Theoretical models predict a population of soft and quasi-localized non-Goldstone modes following a power law that is subdominant with respect to the Goldstone sector. We show that the non-Goldstone sector can be efficiently probed at any system size by employing a random pinning protocol that destroys spatial translational invariance symmetries and thus removes phonons from the spectrum[1]. Moreover, we show that non-Debye modes dominate the low-frequency spectrum in supercooled liquids equilibrated at parental temperatures close to the dynamical transition temperature. Finally, we make in contact the emerging of non-Goldstone modes with the growing of dynamical heterogeneous regions [2].

[1] L. Angelani, M. Paoluzzi, G. Parisi, and G. Ruocco, PNAS **115**, 8700 (2018).

[2] M. Paoluzzi, L. Angelani, G. Parisi, and G. Ruocco, arxiv.org/abs/1901.09796 (2019).

STUDY OF THE CONNECTION OF DISORDER AND ENERGY LANDSCAPE IN GLASSES USING HYPERAGED AMBER

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The way structure and dynamics of amorphous materials relate to their thermodynamic metastability is one of the current challenges for the glass transition understanding. A major impediment to the experimental study is the limited range of stability accessible on the laboratory timescale. Fossil amber represents a unique opportunity for investigating the effect of extreme stabilization being a glass which has been exploring its energy landscape for more than 110 Myears. In order to study the link between the structural and vibrational properties of the glass and its potential energy landscape, we characterize fossil amber by means of a combination of x-ray scattering techniques before and after an annealing treatment that erases its thermal history and rejuvenate it. Specifically, we find that hyperaging induces a depletion of the vibrational density of states in the THz region, also ruling the sound dispersion and attenuation properties of the corresponding acoustic waves. Moreover, we observe that the amber stabilization is accompanied by homogeneous densification, different in nature from that caused by hydrostatic compression. Our results can be rationalized within the fluctuating elasticity theory, revealing that upon approaching the bottom of the potential energy landscape the elastic matrix becomes increasingly less disordered, though retaining the vibrational anomalies characteristic of the glassy state.

STRUCTURE AND SELF-ASSEMBLY OF BIOMOLECULES

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Recently, in the field of bio-materials, the non-covalent self-assembly of simple peptide based molecules has gained increasing attention for the formation of nanostructured, biologically functional materials.

Our work concerns the modeling of small biological molecules, where the self-assembly propensity and the conformational properties, are studied through all-atom Molecular dynamics simulations using an explicit solvent model. A very common but of particular interest peptide, is diphenylalanine, FF. Our findings reveal a strong self-assembling propensity of FF in water in contrast to its behavior in methanol. We quantify the interaction between two isolated peptides dissolved in water/methanol through the calculation of a potential of mean force. Pair radial distribution functions between FF peptides, as well as the number of hydrogen bonds are calculated, providing measures of the self-assembly of peptides in the two solvents. Our results are in qualitative agreement with experimental observations. Furthermore the effect of graphene on the formed structures is examined. Atomistic details about the conformational preferences, the orientation of peptides with respect to the surface and the effect of concentration of graphene nanoparticles in water are presented. This detailed information provides useful insight into the mechanism of aggregate deconstruction due to the presence of graphene as well as, the way that peptides hinder the stacking among graphene flakes in water.

POLYMER GRAPHENE NANOSTRUCTURED MATERIALS: AN ATOMISTIC SIMULATION STUDY

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Polymer/graphene nanostructured systems are hybrid materials, which have attracted great attention the last years both for scientific and technological reasons. The aim of our work is to examine spatial and dynamical heterogeneities of graphene based polymer nanocomposite systems and to provide information about their properties for various (edge group functionalized) graphene sheets. Systems with graphene sheets of different sizes have been simulated at the same graphene concentration ($\sim 3\%$). Pristine graphene and two types of functionalized graphene have been simulated in two different polymer matrices, (polyethylene, PE) and (polyethylene oxide, PEO). Systems are studied through detailed atomistic Molecular Dynamics (MD) simulations.

The density of the polymer around the graphene sheet depends on the distance from the surface. An analysis of the PE chain conformations, based on the calculation of the distribution of the torsional angles, in different distances from graphene, reveals trans-enriched configurations, in comparison to the bulk polymers. Therefore in the adsorbed interfacial region, the chains preferably adopt more extended. Similar behavior is observed for PEO. Concerning local dynamic properties of polymer chains, strong dynamical heterogeneities are reported. The effect is more pronounced in the system with the carboxylated sheet. The slowest monomers are observed around the edges of the carboxylated graphene sheet.

ON THE VISCOELASTIC RESPONSE OF SEMIFLEXIBLE NETWORKS

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From the theoretical and computational point of view, methods to evaluate the mechanical response of semiflexible filaments networks are known since almost two decades [1]. However, only now those methods were extended to describe the full viscoelastic response of networks and were applied in the study of the formation of the peptide gels [2]. In contrast to the usual approaches, which are based on continuous/effective descriptions of the elastic media and are limited to length scales much larger than the their smallest structures (e.g., proteins or peptides), our mesoscopic/multi-scale approach provide a novel approach that might lead to new theoretical and computational developments for the characterization of the microrheology of gel-like semisolids materials.

[1] C.P. Broedersz and F.C. MacKintosh, *Rev. Mod. Phys.* **86** 995 (2014).

[2] L.G. Rizzi *et al.*, *Soft Matter* **12** 4332 (2016).

KINETICS ASPECTS OF THE FORMATION OF QUASICRYSTALS

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Quasicrystals are crystalline solids which present orientational but not translational symmetries, and can be observed in a wide range of systems including metallic compounds and colloidal patch particles. Despite of many theoretical and experimental advances in study of such materials, there are still elusive aspects related to their formation and growth. Here we present a simple two-dimensional coarse-grained model for a quasicrystalline structure and study its formation by using kinetic Monte Carlo simulations. This approach allows one to determine several physico-chemical quantities, including the growth probabilities, the critical nucleus size, and the overall nucleation rates. Our simulations provide a simple way to explore the mechanisms involved in the formation of quasicrystals for different concentrations of specimens with different functionality. Thus, the study we present here may provide experimentalists a way for the rational design of such materials with applications in nanotechnology.

DYNAMICAL PROPERTIES OF MAGNETIC GRANULAR MATTER ANALYZED BY DDM

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Applying an unsteady magnetic field on a 2D non-vibrated magnetic granular system induces a random motion on the grains with characteristics analogous to that of molecules in a fluid state. The applied field is generated by the superposition of a constant field and a collinear sinusoidal one. The system reaches quasi-steady-states in which the effective granular temperature is proportional to the amplitude of the applied field. We study the dynamics of the particles at different concentrations and its effect on its movement and interaction between particles.

SIMULTANEOUS DIELECTRIC AND NEUTRON SPECTROSCOPY ISOCHRONAL SUPERPOSITION, AN ISOMORPH TEST

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By combining dielectric spectroscopy (DS) and neutron scattering (NS) in our newly developed high-pressure DS-NS cell [1], we show that both the fast and slow dynamics in simple glass-forming liquids along isochrones, i.e. constant relaxation time $\tau_\alpha(T, P)$, is invariant as predicted by isomorph theory. Experiments were carried out at Institut Laue-Langevin using DS and neutron backscattering from IN16B accessing nanosecond dynamics and neutron time-of-flight from IN5 accessing picosecond dynamics [2,3].

Dynamics in real glass-forming liquids is rich and includes a large range of dynamical processes taking place on different timescales. While the main dynamical feature is the α -relaxation, there is no common understanding yet of what governs the timescale and the spectral shape of the relaxation. It has several times been suggested that there is a close connection between the fast and slow dynamics, even though they differ in timescales by ten or more orders of magnitude.

A recent theoretical development in the physics of liquids, the isomorph theory, rationalises this [4]. The fundamental prediction of the isomorph theory is the existence of isomorphs, i.e. curves in the phase diagram along which all dynamical phenomena and structure are invariant. We can identify possible isomorphs by the isochrones.

We investigate the dynamics with NS on pico- and nanosecond timescales in combination with DS for three liquids along the glass transition isochrone, i.e. $\tau_\alpha = 100$ s [2], and along faster isochrones with the alpha relaxation on nanosecond timescale [3]. We show isomorphs for the van der Waals liquids, i.e. both vibrations and fast relaxations are invariant along the glass transition, and how scaling breaks down for a complex H-bonded liquid.

[1] A. Sanz *et al.*, *Rev. Sci. Instrum.* **89**, 023904 (2018).

[2] H.W. Hansen *et al.*, *Nat. Comm.* **9**, 518 (2018).

[3] H.W. Hansen *et al.*, *J. Phys. Chem* **149**, 214503 (2018).

[4] J.C. Dyre, *J. Phys. Chem. B* **118**, 10007 (2014).

EXAFS AND REVERSE MONTE CARLO ANALYSIS TO REVEAL THE ANOMALOUS BEHAVIOR OF Nb₃Sn IN TEMPERATURE AND PRESSURE

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The A15 phase Nb₃Sn compound is presently the leading material for high field magnet application (CERN LHC Luminosity Upgrade, coils for the ITER project). In these contexts, the great stress to which the material is subjected causes a degradation of the superconducting properties and make it necessary to shed deeper light on the relationship among the atomic structure, electronic transport and environmental parameters such as temperature and pressure. Recently synchrotron radiation XRD experiments have detected an anomalous behavior in the P-V (around 5-10 GPa) and V-T (around 200K) curves but the lack of crystallographic (long range) structural transition pushed to search for local structure effects related to such anomaly. Here we present results of Nb K-edge EXAFS measurements as a function of temperature (in the 10-300K range) and hydrostatic pressure (up to 26 GPa). The EXAFS data analysis carried out via Reverse Monte Carlo method demonstrate a peculiar trend of Nb-Nb nearest neighbor distances that progressively assume a bimodal shape above 5-9 GPa. Inspection of RMC atomic models suggests a dimerization of Nb-chains likely representing the local structure counterpart of the crystallographic anomaly observed in the P-V curves. PDF measurements also give a complete description of pressure induced structural effects. These findings provide novel insight that must be considered in order to improve the knowledge about these important superconductors.

MODE-COUPLING THEORY OF THE GLASS TRANSITION FOR COLLOIDAL LIQUIDS

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We present a derivation of a microscopic theory for the glass transition of a colloidal liquid of hard spheres confined between two parallel flat walls. The theory only requires the equilibrium density profile and the static structure factors as input. Starting with the microscopic motion of the colloids we use the Zwanzig-Mori projection operator formalism to derive equations of motion for generalized matrix-valued correlation functions. In the case of colloidal particles the microscopic dynamics is Brownian motion rather than Newtonian dynamics. To close the equations, suitable mode-coupling approximations (slowing down of the dynamics due to the caging by neighboring particles) are used. Since the geometry lacks translational invariance perpendicular to the walls, the memory kernel naturally splits into components parallel and perpendicular to the walls.

BRILLOUIN SCATTERING OF NANOPARTICLES AND THEIR AGGREGATES IN PHONONIC CRYSTALS. SIZE DEPENDENT T_g

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Brillouin light scattering allows to observe the acoustic vibrations of a particle with a diameter in the range 100–1000 nm in the frequency range of a few GHz. When the particles are organized in a cluster, the vibration of a single isolated particle evolves in phonon bands with frequency dispersion. The interaction between pairs of particles determines the shape of the phonon bands, allowing the measurement of surface dynamics. By measuring the temperature-dependent vibrational modes of polystyrene nanoparticles, we identify the glass-transition temperature and calculate the elastic modulus of individual nanoparticles as a function of particle size and chemistry. Evidence of surface mobility is inferred from the observation of a softening temperature, where the temperature dependence of the fundamental vibrational frequency of the nanoparticles reverses slope below the glass-transition temperature.

OVERCHARGING AND REENTRANT CONDENSATION OF THERMORESPONSIVE IONIC MICROGELS

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Understanding the mechanism driving polyelectrolyte–colloid complexation and nanoparticle adsorption onto oppositely charged surfaces still represents a fundamental problem of great interest and many studies have been published [1–3]. Although these phenomena have been observed in a variety of colloidal mixtures, reported works dealt with fixed charge density. Thermoresponsive microgels, whose synthesis is initiated by charged groups, are characterized by a thermodynamic volume phase transition (VPT) giving the opportunity to tailor adsorption of polyelectrolytes [4] (PE) or nanoparticles (NP) by changing temperature. Indeed, by controlling microgel volume, VPT affects microgel charge density and can enhance electrostatic PE/NP adsorption.

We have investigated the complexation of thermoresponsive ionic PNIPAM microgels with oppositely charged biopolymers and model nanoparticles by different experimental techniques. We show that microgel VPT triggers polyion adsorption only if PE chains are short enough and always determines the onset of microgel reentrant condensation for increasing PE or NP concentrations. Microgels behave as strongly charged colloids only at $T > VPT$, where they phase separate in proximity of the isoelectric point, while their stability stays unaffected by PE or NP adsorption at lower temperatures.

[1] P. Sens and J.F. Joanny, *Phys Rev Lett.* **84**, 4862 (2000).

[2] M. Muthukumar, *Chem Phys* **86**, 7230 (1987).

[3] A. Dobrynin *et al.*, *Phys Rev Lett.* **84**, 3101 (2000).

[4] S. Sennato *et al.*, *Soft Matter* **14**, 4110 (2018).

PREDICTING SCALING PROPERTIES FROM INDIVIDUAL CONFIGURATION

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Some liquids, termed Roskilde simple liquids, have curves in their thermodynamics phase diagram with invariant dynamics and structure. These curves are known as "isomorphs" [1]. Isomorph theory provides a theoretical explanation for the experimentally observed density scaling [2].

Isomorphs can be identified using the following procedure : At a given state point the exponent γ can be calculated from the thermodynamics fluctuations, and $\gamma = (\partial \ln T / \partial \ln \rho)_{S_{ex}}$ is used to identify a new state point on the isomorph [1]. This method works well but requires small density changes in each step.

Here we present a new method for identifying isomorphs, which is based on the invariance of forces in reduced units along the isomorph. One of the advantages of the new method is that a single configuration can be used to generate an isomorph. We demonstrate that, implementing this approach on both atomic and small molecular models determines proper isomorphs and it even predicts the so-called "pseudo-isomorphs" [3].

[1] N. Gnan *et al.*, J. Chem. Phys. **131**, 234504 (2009).

[2] L. Böhling *et al.*, New J. Phys. **14**, 113035 (2012).

[3] E. Olsen *et al.*, J. Chem. Phys. **145**, 241103 (2016).

GLUONIC AND REGULATORY SOLVENTS: FROM CO-NONSOLVENCY IN POLYMERS TO RNA DROPLETS

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generic theoretical concept for phase segregation of polymers in the presence of multi-component selective solvents is presented. Phase separation is caused by non-specific attractive interactions between the polymers and a smaller component in the solution instead of repulsion between monomers and solvent molecules. We call the component which adsorbs on the polymers and thus causes condensation "gluonic". It is shown that a discontinuous phase transition from a diluted or from a semi-diluted state to the condensed state takes place if the fraction of the gluonic component is increased. The origin of the discontinuous transition even in the absence of translation entropy of the chains is the appearance of higher-order negative virial coefficients in the free energy. The location of the phase coexistence can be shifted and tuned by influencing the binding efficiency of the gluonic component. This is achieved by introducing a regulatory component to the solution. The latter can bind to the polymer and thus block monomers from the interaction with the gluonic component. In this way switching of polymer state from dissolved to condensed can be controlled without changing the chemical properties of the polymer-solution-system. Applications of this model range from co-nonsolvency in synthetic polymers, to polymer-nanoparticle systems, to biological systems such as the formation of protein-RNA droplets.

[1] J.-U. Sommer, *Macromolecules* **51**, 3066 (2018)

[2] J.-U. Sommer, *Macromolecules* **50**, 2219 (2017)

ENGINEERING OF FRUSTRATION IN COLLOIDAL ARTIFICIAL ICES REALIZED ON MICROFEATURED GROOVED LATTICES

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Frustration, i.e. the impossibility of minimising competing interactions, underpins the complex and often unpredictable behaviour of many physical and biological systems. Artificial spin-ice systems, namely lattices of interacting single domain ferromagnetic islands, have been used to date as microscopic models of frustration induced by lattice topology, allowing for the direct visualization of spin arrangements and textures. However, the engineering of frustrated ice states in which individual spins can be manipulated in situ and the real-time observation of their collective dynamics remain both challenging tasks. Inspired by recent theoretical advances, we realize a colloidal version of an artificial spin ice system using interacting polarizable particles confined to lattices of bistable gravitational traps. We show quantitatively that ice-selection rules emerge in this frustrated soft matter system by tuning the strength of the pair-interactions between the microscopic units. Via independent control of particle positioning and dipolar coupling, we introduce monopole-like defects and strings and use loops with defined chirality as an elementary unit to store binary information

TIME CORRELATION FUNCTIONS OF SIMPLE LIQUIDS: A NEW INSIGHT ON THE UNDERLYING DYNAMICAL PROCESSES

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Extensive molecular dynamics simulations of liquid sodium have been carried out to evaluate correlation functions of several dynamical quantities. We report the results of a novel analysis of the longitudinal and transverse correlation functions obtained by evaluating directly their self- and distinct contributions at different wavevectors k . It is easily recognized that the self-contribution remains close to its $k \rightarrow 0$ limit, which turns out to be exactly the autocorrelation function of the single particle velocity. The wavevector dependence of the longitudinal and transverse spectra and their self- and distinct parts are also presented. By making use of the decomposition of the velocity autocorrelation spectrum in terms of longitudinal and transverse parts, our analysis is able to recognize the effect of different dynamical processes in different frequency ranges.

IN SILICO MODELLING OF MICROGEL PARTICLES

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Thermoresponsive microgels are soft colloids which have been recently widely applied in experiments and in several applications, because of their tunable size which can be easily and reversibly changed *in situ*. Despite the large experimental interest, theory stands behind, as models lack a comprehensive description in terms of the internal polymeric nature of the microgels, which is fundamental to correctly describe their elasticity and deformability, especially at high densities [1].

We are now able to provide novel theoretical insights in this respect, thanks to a new model that reproduces *in silico* realistic PNIPAM microgels. To this aim, we assemble the microgel network using bi- and tetra-valent patchy particles confined within a spherical cavity. We then fix the topology by switching on a bead-spring model [2]. The computational protocol is validated, in the first place, by comparing the calculated form factors to the ones obtained experimentally. Secondly, we verify that designed and experimental microgels with equal crosslinks ratio undertook the same swelling behavior. Further improvements have allowed to introduce in the model a coarse-grained explicit solvent [3]. This allows us to simulate the flattening of the microgels at liquid-liquid (e.g. oil-water) interfaces [4]. The newly designed protocol paves the way to the calculation of the single-particle elastic properties and of the effective interactions acting between microgels [5].

[1] A. Lyon and A. Fernandez-Nieves, *Annu. Rev. Phys. Chem.* **63**, 25-43 (2012).

[2] N. Gnan *et al.*, *Macromolecules* **50** (21) (2017).

[3] A. Ninarello *et al.*, arXiv:1901.11495.

[4] F. Camerin *et al.*, *Sci. Rep.* **8**, 14426 (2018).

[5] L. Rovigatti *et al.*, arXiv:1808.04769.

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