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Dipartimento di
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XVII International Workshop on COMPLEX SYSTEMS

9–12 March, 2026 – Andalo (Trento)

Book of abstracts

Contents

Part I

Programme

Monday, 9 March 2026

16.00

OPENING

Giacomo Baldi, Raffaello Potestio, and Marco Zanatta

SPECIAL SESSION:
IN MEMORY OF ULI BUCHENAU

Chair: Giacomo Baldi

16.10 Aldo Fontana
Uli Buchenau

16.20 Miguel Ángel Ramos
Uli Buchenau and the soft potential model

16.40 Alexei P. Sokolov
The journey with Uli: from fast dynamics to structural relaxation

17.00 Stefanie Buchenau
Memories of my father

17.10 **COFFEE BREAK**

Chair: Beatrice Ruta

17.40 Haiyang Bai
Breaking the vitrification limitation of monatomic metals

18.00 Eloi Pineda
Evolution of structural dynamics in metallic glassformers during glass transition and physical aging

18.20 Rui Zhao
Observation of glass transition occurring on surfaces of metallic glasses

20.00 **DINNER** at Hotel La Bussola

Tuesday, 10 March 2026

Chair: Jeppe Dyre

9.00 Peng Luo
  Emergence of a long-range interfacial relaxation in supercooled liquids

9.20 Giulio Monaco
  At the crossover between quasi-localized dynamics and diffusion in deeply supercooled liquids

9.40 Gerhard Jung
  Numerical investigation of the equilibrium Kauzmann transition in a two-dimensional atomistic glass

10.00 Nils Holle
  Collective structural relaxation in glassy antimony

10.20 Francesco Dallari
  Mechanisms of the X-ray induced fluidization in inorganic glasses

10.40 **COFFEE BREAK**

Chair: Simone Napolitano

11.10 Federico Caporaletti
  Can slow liquid dynamics release stress in confined polymers?

11.30 Catalin Gainaru
  Revised MN rules for relaxation and transport phenomena in liquids and polymers

11.50 Felix Lehmkühler
  XPCS in soft matter: From sub-microsecond nanogel collapse to multi-decade colloidal gelation

12.10 Jeppe C. Dyre
  The material-time concept in physical aging

12.30 Thomas Franosch
  Static and dynamic properties of modulated colloidal monolayers

12.50 **LUNCH BREAK**

Chair: Thomas Schrøder

16.00 Simone Capaccioli
  Complex water dynamics in aqueous mixtures spanning a wide concentration-temperature-pressure range

16.20 Sandra Krüger
  Low-temperature water dynamics in confinement and mixtures

16.40 Ari Paavo Seitsonen
  On the importance of the long-range, electro-static interaction in water

17.00 Andrea Corradini
  Hunting for the critical point: the twelve anomalies of liquid tellurium

17.20 - 18.50
POSTER SESSION
with cheese and wine tasting

20.00 **DINNER** at Hotel La Bussola

Wednesday, 11 March 2026

Chair: Giulio Monaco
9.00 Misaki Ozawa
Creating bulk ultrastable glasses by random particle bonding
9.20 Cristian Rodriguez-Tinoco
Real-time observation of the heterogeneous relaxation of a glass
9.40 Lara Piemontese
Temperature-dependent relaxation pathways in a $GeSe_2$ glass: an XPCS study
10.00 Fabio Brugnara
X-ray driven amorphous-amorphous transitions in v-GeO_2
10.20 Till Böhmer
The material time of physical aging – and beyond

10.40 **Coffee Break**

Chair: Giancarlo Ruocco
11.10 Hajime Tanaka
Microscopic origin of the boson peak in model glasses
11.30 Walter Schirmacher
The influence of frozen-in stresses on the vibrational excitations in glasses
11.50 Daria Szewczyk
Substitution-driven glassy anomalies in benzene derivatives: the role of methyl and chlorine arrangement
12.10 Anaël Lemaître
The vibrational spectrum of silica: hidden counting rules and microstructural determinants
12.30 Denis Nabari
High-frequency sound attenuation of vitreous silica probed by extreme UV transient grating spectroscopy

12.50 **Lunch Break**

Chair: Raffaello Potestio
16.00 Claudio Maggi
Continuous phase transitions in active particles matter
16.20 Roberto Menichetti
Artificial life of an active droplets system: a quantitative lifecycle analysis
16.40 Foivos Perakis
Coherent X-ray scattering of fluctuations and dynamics in complex systems

17.00 **Coffee Break**

Chair: Walter Schirmacher
17.30 Federico Ricci-Tersenghi
Soft modes in vector spin glass models on sparse random graphs
17.50 Luca Leuzzi
Multiphoton quantum simulation of a generalized dense Hopfield neural network
18.10 Rolf Zeißler
On the role of molecular details in structural relaxation
18.30 Aleksander Krivchikov
Linear low-temperature heat capacity in graphite-derived nanostructures

20.00 **Dinner** at Hotel La Bussola

Thursday, 12 March 2026

Chair: Simone Capaccioli

9.00 Thomas B. Schrøder
Dynamics of viscous liquids and the random barrier model

9.20 Stefano Mossa
Competing length scales and screening in dense electrolytes

9.40 Taras Bryk
Which processes define the propagation of collective excitations in simple and binary liquids?

10.00 Laurence Noirez
When liquids flow on solids: unexpected deep liquid-solid THz coupling

10.20 Jesper Schmidt Hansen
Polarization dynamics

10.40 **COFFEE BREAK**

Chair: Hajime Tanaka

11.10 Minqiang Jiang
Unified theory of phonon in solids with phase diagram of non-Debye anomalies

11.30 Matthias Fuchs
On the Euclidean random matrix model of vibrations in glass

11.50 Josep Lluís Tamarit
Unveiling glass-like behavior in molecular crystals with minimal disorder

12.10 Søren Strandskov Sørensen
Decoupling density and disorder effects on the boson peak in metal-organic frameworks

12.30 Mariangela Ruggeri
Emergent glass-like dynamics and low-energy excitations in cesium halide perovskites

12.50 **LUNCH BREAK**

Chair: Felix Lehmkühler

16.00 Johannes Möller
Photon correlation methods at the MID instrument at European XFEL

16.20 Noemi D'Abbondanza
Development of heterodyne brillouin microscopy

16.40 Peihao Sun
Setup combining fast scanning calorimetry with X-ray total scattering

17.00 **COFFEE BREAK**

Chair: Claudio Maggi

17.30 Lorenzo Rovigatti
A phase-field model for solutions of DNA-made particles

17.50 Greta Grassmann
A minimal molecular model for probing the role of RNA in protein condensates

18.10 Carolina Palombo
Polycatenane assembly with TopoII in toroidal confinement

18.30 Simone Scalise
A microfluidic device for single-cell analysis of T-cell growth and proliferation

20.00 **GALA DINNER** at Hotel La Bussola

Friday, 13 March 2026

Chair: Thomas Franosh

9.00 Mattia Miotto

Symmetry-breaking processes drive multicellular rosette morphogenesis

9.20 Simone Napolitano

Tiny movements, big changes: When slow dynamics decides how fast liquids and glasses relax

9.40 Alessandro Martinelli

Hierarchical dynamics and time-length scale superposition in glassy suspensions of ultra-low crosslinked microgels

10.00 Raffaele Pastore

Fickian yet non-Gaussian: a new paradigm for diffusion in glassy materials

10.20 Andrij Trokhymchuk

Complex assemblage of a simple system: bimodalities of local ordering in 2D hard disks

10.40 **Coffee Break**

Chair: Miguel Ángel Ramos

11.10 Stephen Elliott

Chiral crystallization of amorphous tellurium

11.30 Kohsaku Kawakami

Relevance between molecular cooperativity and nucleation of organic glasses

11.50 Michele Magnozzi

Exploring in real time the thermal annealing of amorphous mixed oxide coatings

12.10 Mattia Biesuz

Relaxation phenomena during chemical tempering of soda-lime silicate glass

12.30 Marta Ruiz

Thermal stability of organic semiconductor thin film glasses by local changes in spontaneous orientation polarization

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12.50 - 13.00

Conclusive remarks

Posters

Abolfazl Ahmadirahmat
Light-induced caging in colloidal suspensions

Giacomo Baldi
Effect of glass stability on the low frequency vibrations of vapor deposited glasses.

Beatrice Baraldi
In-situ XRD tracking of structural changes in metallic glasses during thermal scans

Simone Capaccioli
Calorimetric analysis of deposited amorphous GeTe and its relevance for phase-change materials applications

Federico Caporaletti
Predicting the crystal growth rate at the surface of molecular glasses

Domenico Caudo
Coupling growth strategies to organelle partitioning noise explains generation-dependent biases in cell proliferation

Gabriel Cuello
Extraction of real-space correlation functions from neutron total scattering experiments

Fausta Desantis
Monte Carlo-based design of an inhibitory peptide to impede pathogenic dimerization in a misfolded antibody light chain

Lorenzo Di Rienzo
Computational approaches to describe biomolecular interactions: exploring their implications in molecular design

Jepsinraj Kakkuzhiyulla Parambath
NMR studies of water and ion dynamics in synthetic fluoro-hectorite

Francesco Pecorella
Description of the complete phase diagram of GeTe with a single machine learning potential

Eloi Pineda
Quantitative assessment of physical aging on the dynamical heterogeneity of amorphous alloys: Insight from stress relaxation

Robert Schlothauer
A mode-coupling theory of the glass transition for polydisperse systems

Finn Wolter
NMR Study on the dynamics of ice in bulk and confinement

Ronen Zangi
Modeling liquid-liquid phase diagrams of thermoresponsive materials

Simone Ziglio
Temeprature-dependent structural evolution in a strong glassformer: the case of v-GeO_2

Xu Zongrui
Revealing hierarchical relaxation pathways during physical aging of metallic glasses

Part II

Talks

ULI BUCHENAU AND THE SOFT POTENTIAL MODEL

Miguel Ángel Ramos

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In this talk, dedicated to the memory of my colleague, mentor, and friend Uli Buchenau, I will combine personal recollections of his scientific life and his uniquely generous character with his decisive role, over several decades, in the development and application of the Soft-Potential Model – one of the most widely used frameworks for understanding low-energy excitations and low-temperature properties of glasses and amorphous solids.

Uli Buchenau was an active participant in the Andalo workshops essentially from the beginning, attending the vast majority of them. In this special session in his honor, I will also attempt to explain the motivations and the underlying reasoning behind his adoption of the Soft-Potential Model, inspired by his experimental results on inelastic neutron scattering in glasses, and how he progressively refined the model to make it more useful for experimental physicists – a trajectory I was fortunate to follow alongside him for most of the time.

The journey with Uli: from fast dynamics to structural relaxation

Alexei P. Sokolov

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I will start the talk with a few personal memories of working with Uli Buchenau and learning from him neutron scattering. It was very encouraging and rewarding experience. Next, I will discuss the fast dynamics in glass forming systems, including the boson peak and fast picosecond relaxation where Uli's works left significant impact. The focus will be on collective dynamics and coherent neutron scattering, medium range order and elastic constants heterogeneities. Then I will discuss the puzzling correlations between fast dynamics and temperature dependence of structural relaxation first discovered by Zorn and Buchenau in 1992 [1]. Understanding this puzzling relationship between the fast and slow dynamics separated by more than 12 decades in time remains a challenge. This talk will summarize several ideas connecting parameters controlling the fast dynamics to parameters affecting the energy barriers controlling structural relaxation.

[1] U. Buchenau and R. Zorn, Europhys. Lett. **18**, 523 (1992).

Breaking the vitrification limitation of monatomic metals

Haiyang Bai[1,2], X. Tong[2], Y.-E. Zhanga[2], H. Ke[2], J. Zhou[3], and W. Wang[1,2]

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The question of whether all materials can solidify into the glassy form proposed by Turnbull half a century ago remains unsolved. Some of the simplest systems of monatomic metals have not been vitrified, especially the close-packed face-centered cubic metals. Here we report the vitrification of gold, which is notoriously difficult to be vitrified, and several similar close-packed face-centered cubic and hexagonal metals using a method of picosecond pulsed laser ablation in a liquid medium. The vitrification occurs through the rapid cooling during laser ablation and the inhibition of nucleation by the liquid medium. Using this method, a large number of atomic configurations, including glassy configurations, can be generated simultaneously, from which a stable glass state can be sampled. Simulations demonstrate that the favorable stability of monatomic metals stems from the strong topological frustration of icosahedra-like clusters. Our work breaks the limitation of the glass-forming ability of matter, indicating that vitrification is an intrinsic property of matter and providing a strategy for the preparation and design of metallic glasses from an atomic configuration perspective.

EVOLUTION OF STRUCTURAL DYNAMICS IN METALLIC GLASS-FORMERS DURING GLASS TRANSITION AND PHYSICAL AGING

Eloi Pineda[1], Z. Xu[1], Y. Duan[2], and M. Frey[3]

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The structural dynamics of liquids and glasses comprise a broad spectrum of relaxation modes. How this spectrum evolves through temperature and time is a key knowledge to understand important technological aspects of glasses, such as the crystallization rates, the aging and rejuvenation processes and the mechanical behavior. In this talk, I will present different experimental observations of the structural dynamics in metallic glass-formers which provide information on how the timescales and heterogeneity of the relaxation spectrum evolves with temperature and time. By mechanical experiments, the dynamic spectrum can be reconstructed from different types of probes. The spectrum is found to be constituted by a wide, high-frequency wing of reversible, inelastic deformation modes, which determine the rheological behavior, stress relaxation and mechanical memory effect of these materials. I will show how all these phenomena can be interpreted within the linear viscoelasticity framework and the relation between the mechanical spectrum and the thermodynamic evolution during structural relaxation. By scattering of coherent X-rays, using the X-ray Photon Correlation Spectroscopy technique, we can experimentally determine the intermediate scattering function for times going from milliseconds to hours, which are the relevant timescales during the glass transition. I will discuss how we can interpret this microscopic information and its relation with the macroscopic behavior.

OBSERVATION OF GLASS TRANSITION OCCURRING ON SURFACES OF METALLIC GLASSES

Rui Zhao, J. Yu, L. Shen, P. Luo, H. Bai, and W. Wang

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The glass transition temperature (T_g) of the surficial layer of some glasses can be substantially lower that of bulk counterparts. This phenomenon determines the performance of glassy materials under nanoscale and enables the formation of ultra-stable glasses. Despite its significance, how and to what extent T_g is depressed when approaching the surface remains unknown for metallic glasses. Here, we successfully observe the occurring of glass transition in surficial region within thickness of only $1-5$ nm of various metallic glasses, by tracing the evolution of surficial adhesion force during heating. The transition from rigid glass to viscous liquid induce abrupt increase of adhesion force, allowing the quantitative determination of surficial T_g. Remarkably, the depression of T_g of metallic glasses reach $40-80$ K, comparable to that observed in soft polymer materials. It is further revealed that the degree of T_g depression near surface relative to the corresponding bulk materials is negatively correlated with the fragility of MGs, which is also confirmed by computer simulations.

EMERGENCE OF A LONG-RANGE INTERFACIAL RELAXATION IN SUPERCOOLED LIQUIDS

Peng Luo[1], P. Wen[1], B. Ruta[2], H. Bai[1], and W. Wang [1]

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Interfacial effects are known to influence the dynamics of supercooled liquids, but they are generally believed to be confined to molecular or nanometer length scales. Here we report the emergence of a distinct, long-range interfacial relaxation in a wide range of supercooled liquids — including oxide (B_2O_3), ionic ($Ca_2K_3(NO_3)_7$), and polymeric (polycarbonate) systems — in contact with rigid boundaries. Using dynamic mechanical analysis, we observe an additional relaxation process that is absent in non-contact samples and corresponds to relaxation times more than two orders of magnitude slower than the bulk response, together with a markedly stronger deviation from Arrhenius temperature dependence. Remarkably, this interfacial relaxation remains clearly detectable in millimeter-thick samples. Thickness-dependent measurements further reveal that the affected interfacial layer extends up to approximately 30 μm from the boundary. The observation of a micrometer-scale inter-facial relaxation uncovers an unexpected long-range influence of rigid boundaries on liquid dynamics, with potential implications for controlling material properties even at macroscopic length scales.

AT THE CROSSOVER BETWEEN QUASI-LOCALIZED DYNAMICS AND DIFFUSION IN DEEPLY SUPERCOOLED LIQUIDS

F. Caporaletti[1], S. Capaccioli[2], D. Bessas[3], A.I. Chumakov[3], A. Martinelli[4], F. Dallari[5], and **Giulio Monaco**[5]

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[4] Laboratoire Charles Coulomb, Université de Montpellier, CNRS, Montpellier, France.
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The Johari-Goldstein β_{JG}-relaxation process [1] is active in deeply supercooled liquids and glasses, where it plays an essential role in several relevant physical properties. The relaxation can be considered a precursor of the glass transition in time and temperature: it is faster than the structural (or α) relaxation by many decades and remains active in the glass [1,2]. This process has been traditionally studied mainly using dielectric and mechanical spectroscopy techniques, which point toward a quasi-localized nature. Direct experimental information on its microscopic properties remains scarce. A wavevector-resolved x-ray-based technique, nuclear-resonance time interferometry [3-5], is here used to obtain information on this relaxation in a hydrogen-bonded liquid, 5-methyl-2-hexanol. Our investigations address the microscopic density fluctuations in the proximity of the crossover temperature where the β_{JG}-relaxation decouples from the structural relaxation. Our approach provides the characteristic mean-squared displacement related to the process elucidating its relationship with the α-relaxation and its role as an initiator of cage-breaking events [4-5]. Our results thus provide a novel picture of the role of the Johari-Goldstein relaxation in the dynamics of supercooled liquids.

[1] G.P. Johari & J. Goldstein, J. Chem. Phys. **53**, 2372–2388 (1970).
[2] K.L. Ngai, *Relaxation and Diffusion in Complex Systems* (Springer, 2011).
[3] F. Caporaletti *et al.*, Nat. Comm. **12**, 1867 (2021).
[4] F. Caporaletti *et al.*, J. Mol. Liq. **383**, 122107 (2023).
[5] F. Caporaletti *et al.*, in preparation (2025).

NUMERICAL INVESTIGATION OF THE EQUILIBRIUM KAUZMANN TRANSITION IN A TWO-DIMENSIONAL ATOMISTIC GLASS

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[3] Laboratoire de Physique de l'Ecole Normale Supérieure, ENS, Paris, France.
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More than seventy years ago, Kauzmann posed a fundamental question concerning the glass transition: If we could cool liquids in experiments infinity slowly would there exist a critical temperature at which an ergodicity-breaking phase transition occurs [1]? Despite centuries of efforts, this question has still not been answered since making theoretical progress in two or three dimensions is challenging, while experimental and numerical limitations hinder direct observation of this putative Kauzmann transition.

In my talk I will present a strategy to overcome this longstanding barrier by combining three advanced Monte Carlo methods to sample the equilibrium structures of a two-dimensional atomistic glass-forming liquid down to $T \to 0$ across a range of system sizes [2]. I will demonstrate that thermodynamic measurements provide strong evidence that the system undergoes a Kauzmann transition at a temperature that appears to vanish for larger systems. This transition is towards an ideal glass state characterized by a complex energy landscape with a hierarchical organization of low-lying states.

Finally I will give an outlook on how our results could serve as a foundation for future simulation work on larger systems, three-dimensional materials, and more complex glass-forming models to elucidate the nature of the glass state of matter.

[1] W. Kauzmann, Chem. Rev. **43**, 219 (1948).
[2] G. Jung, M. Ozawa, G. Biroli, L. Berthier, arXiv:2507.03590 (2025).

COLLECTIVE STRUCTURAL RELAXATION IN GLASSY ANTIMONY

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Structural relaxation is a ubiquitous phenomenon in glassy materials. For phase change materials (PCMs), it is usually connected to the increase of resistivity over time, which hinders the realization of multi-bit PCM memory for neuromorphic hardware. Here, we show that relaxation in glassy antimony, a single-elemental PCM [1, 2], involves plenty of extended unstable vibrational modes, or "saddle points" in the potential energy landscape. We use a machine-learned interatomic potential [3] trained on density functional theory data to investigate the temperature dependence of instantaneous normal mode spectra [4, 5] in supercooled-liquid and glassy antimony. These spectra probe the potential energy landscape of a system (like a liquid or glass) at a specific moment in time, which allows for unstable modes (imaginary frequencies) due to unrelaxed atomic positions. We find that unstable modes are preferentially located in regions with a low amount of Peierls-like distortion, explaining a density anomaly in the diffusion on short time scales. Our findings are in contrast to descriptions of relaxation based on rearrangements of rather small and independent regions. Instead, they support a picture of complex saddle points where many atoms contribute to individual relaxation events.

[1] M. Salinga *et al.*, Nat. Mater. **17**, 681-685 (2018).
[2] N. Holle *et al.*, Phys. Rev. Lett. **134**, 046101 (2025).
[3] A.V. Shapeev, Multiscale Model. Sim. **14**, 1153-1173 (2016).
[4] S.D. Bembenek and B.B. Laird, Phys. Rev. Lett. **74**, 936 (1995).
[5] W. Schirmacher *et al.*, Proc. Natl. Acad. Sci. U.S.A. **119**, e2119288119 (2022).

MECHANISMS OF THE X-RAY INDUCED FLUIDIZATION IN INORGANIC GLASSES

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In the past decades the brilliance of synchrotron radiation light-sources underwent a tremendous increase opening the way to several new X-ray based techniques together with new phenomena and challenges. A typical obstacle comes from the interaction of intense X-ray beams with matter which can induce unwanted changes in the probed samples. While in organic substances this results in a complete degradation of the system, for inorganic materials, such as oxide glasses, permanent structural modifications appear only at considerable X-ray doses (typically several GGy), but this doesn't mean that the system is unaffected even at lower doses. A series of X-ray Photon Correlation Spectroscopy (XPCS) measurements, revealed that oxide and chalcogenide glasses display dynamics at atomic length-scales activated by the absorbed X-rays and at doses below the ones associated with permanent structural modifications. This beam induced dynamics appears to be a peculiar characteristic of network glasses and can be observed in the correlation functions measured with XPCS experiments as a mechanism competing with thermally activated relaxations. Many aspects of this phenomenon are still unclear but there are indications that it can be linked to more general properties of the glassy state. Combining several experiments, a phenomenological picture is beginning to emerge. In this contribution I will present some recent results on the photo-induced effects on different dose and dose rate regimes in covalently bonded glasses.

Can slow liquid dynamics release stress in confined polymers?

Federico Caporaletti[1,2], J. Mangialetto[1], N. Van den Brande[1], G. Van Assche[1], and S. Napolitano[2]

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Stress in polymers often relaxes on timescales that are decoupled from segmental motions and governed by a nearly constant activation barrier [1–3]. In this talk, I will discuss how these anomalous equilibration pathways can be traced back to collective small displacements (CSD), which do not require the large molecular hops characteristic of segmental dynamics. These subtle molecular rearrangements underpin the slow Arrhenius process (SAP), a relaxation mode observed in the dielectric response of polymers and small organic molecules.

The SAP is active in both the liquid and glassy states. Although it is slower than the α-process in the melt, it becomes the faster process below the glass transition temperature [4–5]. Moreover, SAP is closely linked to high-temperature flow — sharing the same activation barrier — and has been associated with various equilibration kinetics [5-6].

By combining rheology, dielectric spectroscopy, and optical spectroscopy, and by revisiting existing data from the literature, we show that SAP exhibits the same thermal activation barrier as stress relaxation in nanoconfined polymers and shares a characteristic timescale with the enhanced mobility observed at polymer interfaces. These findings suggest that the slow liquid dynamics encoded in SAP may provide an alternative pathway for lowering polymer free energy.

F.C. received an FWO senior postdoctoral fellowship (1262826N) and J.M. received an FWO junior postdoctoral fellowship (1203524N).

[1] M. Chowdhury *et al.*, Phys. Rev. Lett. **109** 136102, (2012).
[2] S. Chandran and G. Reiter, ACS Macro Lett. **8(6)** 646–650, (2019).
[3] H. Yuan *et al.*, Sci. Adv. **8**, eabq5295 (2022).
[4] Z. Song, C. Rodríguez-Tinoco, A. Mathew, and S. Napolitano, Sci. Adv. **8**, eabm7154 (2022).
[5] F. Caporaletti and S. Napolitano, Phys. Chem. Chem. Phys. **26**, 745–748 (2024).
[6] F. Caporaletti *et al.*, Mater. Horiz. (2025).

REVISED MN RULES FOR RELAXATION AND TRANSPORT PHENOMENA IN LIQUIDS AND POLYMERS

Catalin Gainaru[1], H. Singh[2], I. Popov[3], R. Kumar[4], K.S. Schweizer[5], and A.P. Sokolov[1,6]

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Understanding activation barriers controlling structural relaxation in glass-forming liquids, molecular transport and ionic conductivity in amorphous polymers is a grand challenge of fundamental scientific and engineering interest across disciplines. Over decades, intriguing but puzzling empirical correlations between the elementary time scale of activated barrier crossing and the apparent Arrhenius activation energy, the so-called Meyer-Neldel (MN) rules have been discovered in diverse liquids and glasses. Here we formulate and successfully apply a new experimental analysis and an explicitly dynamical theoretical framework which provides an understanding of the origin, validity, and failure of such correlations, that bridge and unify the three fields of structural relaxation, molecular transport, and ionic conductivity in liquids and quenched glasses. Distinct quasi-universal laws are predicted in equilibrated liquids and nonequilibrium glasses, consistent with experiments. Our analysis reveals that even if the relaxation appears Arrhenius over a limited temperature range, the physical activation barrier is generally temperature dependent in polymeric systems even below glass transition temperature. In addition, we show that the approximate validity of classical MN rules hinges on a linear temperature dependence of this barrier and the temperature range probed in experiments. Our findings are relevant for controlling the activation barrier in functional soft polymeric materials relevant to molecular separations, barrier coatings, and charge transport, and provide new constraints on theoretical understanding of the mechanism underlying slow activated dynamics in glass-forming condensed matter.

XPCS in Soft Matter:
From Sub-Microsecond Nanogel Collapse to Multi-Decade Colloidal Gelation

Felix Lehmkühler

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Recent advances in X-ray photon correlation spectroscopy (XPCS) combined with novel detectors and latest generation storage ring and FEL sources, now enable probing nanoscale dynamics down to microsecond and nanosecond regimes. This talk presents a unified perspective on how these capabilities enhance our understanding of nanoparticle and polymer behavior in complex environments. I will discuss stimuli-responsive nanogels, where megahertz-rate XPCS at the European XFEL revealed sub-microsecond collapse of PNIPAm shells on silica nanoparticles, while reswelling occurred 2–3 orders of magnitude more slowly [1]. High-pressure XPCS further elucidated its phase behavior [2]. Afterwards, I will focus on real-time studies of (a) colloidal gelation, spanning more than 8 decades in time [3,4], and (b) dynamics of polymer-coated nanoparticles in crowded protein solutions, showing nanoscopic viscosity deviations from bulk expectations [5]. Finally, I will discuss first results using event-driven XPCS achieving sub-100 ns resolution [5]. A focus is set on colloidal gelation, building on prior work [5], and the potential of such detection schemes at FEL sources.

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THE MATERIAL-TIME CONCEPT IN PHYSICAL AGING

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This talk presents experimental and simulation data on physical aging, which illustrate and validate the old concept of a "material time" controlling aging. The beautiful idea behind this of Narayanaswamy (1971) [1] is that the highly nonlinear aging phenomenon can be described in terms of standard linear-response theory if time is replaced by material time. One may think of the material time as analogous to the proper-time concept of relativity theory, the time read on a clock following the observer. In the case of a temperature down jump from a state of equilibrium, the clock rate gradually decreases to eventually reach the equilibrium relaxation rate characterizing the final temperature.

We present data confirming this approach to physical aging and relate the material-time concept to the groundbraking triangular relation of Kurchan and Cugliandolo (1994) [2]. The experimental data presented include the first direct test of Narayanaswamy's approach (from accurate dielectrics) [3], as well as light-scattering data establishing "material-time reversibility" [4]. Supplementing this, simulation data will be presented that illuminate a "distance-as-time" interpretation of the material time [5]. The latter data show that aging is controlled by how fast the slowest particles move. This very recently led to the concept of "double percolation" controlling the alpha and beta relaxations of equilibrium (metastable) glass-forming liquids [6].

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STATIC AND DYNAMIC PROPERTIES OF MODULATED COLLOIDAL MONOLAYERS

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Colloidal suspensions provide a powerful platform for liquid-state physics: particle positions are directly accessible, and their softness allows controlled exploration of nonlinear response under strong external fields. Leveraging these advantages, we probe the nonlinear response of a liquid to a spatially periodic field through coordinated experiments, simulations, and theory [1]. We observe pronounced structural changes perpendicular to the modulation direction, with amplitude and symmetry that vary sensitively with the imposed period. The field selectively amplifies locally favored motifs of the unperturbed liquid, enabling access to structural information that remains hidden in conventional scattering.

We further present a mode-coupling theory for modulated liquids [2,3] and map the non-equilibrium phase diagram, including the glass-transition line. A central result is a non-monotonic dependence on the modulation period: in certain parameter regimes the modulation promotes vitrification, while in others it stabilizes the fluid. We attribute this to a competition between local ordering tendencies and compliance with the imposed pattern, which selects preferential structural responses.

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COMPLEX WATER DYNAMICS IN AQUEOUS MIXTURES SPANNING A WIDE CONCENTRATION–TEMPERATURE–PRESSURE RANGE

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Decades of intensive research reveal that supercooled and glassy systems exhibit remarkably similar dynamical features across a wide range of glass-forming materials, including hydrated biomolecules [1]. Although recent studies [2–4] have advanced our comprehension of how water influences solute dynamics over a broad hierarchy of timescales, refining the concepts of plasticization and the "slaving" effect, the specific role of water in shaping emerging dynamic processes remains only partially understood.

In this work, we investigate aqueous mixtures containing small hydrophilic solutes and demonstrate that, beyond a certain concentration, the system undergoes a crossover from solute-dominated dynamics to behavior governed by the hydrogen-bond network. Our analysis focuses on fast processes that are intrinsically linked to structural relaxation: namely, caged molecular dynamics (ps–ns range) and the Johari–Goldstein β relaxation. Finally, we examine how pressure modulates the dynamics of both solute and water components, relating these effects to the strength of intermolecular interactions.

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Low-temperature water dynamics in confinement and mixtures

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In various nanoconfinements and mixtures, a dynamical crossover is observed for supercooled water. This transition gives rise to a low-temperature water process with an activation energy of 0.5 eV and a symmetric dynamic susceptibility [1]. However, the microscopic nature of this process and its relation to the phase behavior and glass transition of bulk water remain unclear. To investigate the characteristics of this process, we employ dielectric spectroscopy and various ^{1}H and ^{2}H nuclear magnetic resonance (NMR) methods for component-selective studies of molecular reorientation and diffusion. We investigate supercoolable dipeptide water mixtures and nonfreezable water in narrow confinements e.g. metal-organic frameworks or silica nanopores. For comparison, we study the water dynamics in confinements and mixtures where partial freezing occurs. We show that ^{2}H stimulated-echo experiments are useful to measure multi-time correlation functions of water. F_2 enables detailed insights into the correlation times and the mechanism of molecular reorientation. For liquid water in dipeptide mixtures and in various confinements, we find quasi-isotropic and strongly nonexponential reorientation even below the dynamical crossover. In addition ^{2}H NMR three-time (F_3) and four-time (F_4) correlation functions allow us to in investigate the origin of the strong nonexponentiality of confined water. They reveal rapid rate exchange incompatible with strictly local low-temperature water dynamics.

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On the importance of the long-range, electro-static interactions in water

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The importance of the long-range, in particular the electro-static interactions, is basic knowledge in polar liquids. Still many of the recent potential models, used in computer simulations of liquid water, are based on local models of the interactions parametrised using machine learning; these kind of Machine Learning Interaction Potentials (MLIPs) have been used in several studies, providing results appearing as satisfactory.

There are recent schemes that include long-range interactions beyond the local ones. One of them is called the Latent Ewald Summation (LES) [1]. It allows the charges being fitted to the energies and forces, without needing the estimation of the atomic "charges" as input parameters to the learning.

Here we investigate the importance the inclusion of the explicit electro-static interactions, using the method LES in MLIPs, in the collective dynamics of liquid water, extending our earlier results [2] to the MLIPs, enabling larger systems and longer simulations. Similar to the results reported in Ref [1] and references therein on the dipole-dipole correlations we find a qualitative error appearing at low wave numbers, or large distances in real space; furthermore we discuss the apparent short-coming in the present implementation of the LES that shows up at the very small wave numbers.

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HUNTING FOR THE CRITICAL POINT: THE TWELVE ANOMALIES OF LIQUID TELLURIUM

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Elemental tellurium is a strong candidate for switching devices in phase change memories, thanks to its ultrafast crystallization kinetics [1]. However, liquid tellurium has proven challenging to model, with molecular dynamics studies struggling to accurately reproduce its experimental liquid structure [2]. Moreover, liquid tellurium shows many thermodynamic anomalies in the undercooled liquid phase, involving the density, isothermal compressibility and intermediate-range structure [3]. Strikingly, the density and isothermal compressibility anomalies are almost identical to those in liquid water, which have been related to the existence of two microscopic states and to a liquid-liquid critical point at positive pressure [4]. Here, we extensively investigate the structure of liquid tellurium with molecular dynamics simulations employing a state-of-the-art machine learning interatomic potential trained on hybrid density functional theory data [5,6]. We show a much better agreement between theoretical and experimental data. Furthermore, we also identify a huge number of structural and electronic anomalies in undercooled liquid tellurium, involving the evolution of chain, ring and cluster statistics, changes in angular and radial correlations and a metal-semimetal transition. This strongly suggests the presence of a liquid-liquid critical point in undercooled tellurium at positive pressure, in a water-like fashion [3].

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Creating bulk ultrastable glasses by random particle bonding

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A recent breakthrough in glass science has been the synthesis of ultrastable glasses via physical vapor deposition techniques. These samples display enhanced thermodynamic, kinetic and mechanical stability, with important implications for fundamental science and technological applications. However, the vapor deposition technique is limited to atomic, polymer and organic glass-formers and is only able to produce thin film samples. Here, we propose a novel approach to generate ultrastable glassy configurations in the bulk, via random particle bonding, and using computer simulations we show that this method does indeed allow for the production of ultrastable glasses. Our technique is in principle applicable to any molecular or soft matter system, such as colloidal particles with tunable bonding interactions, thus opening the way to the design of a large class of ultrastable glasses.

REAL-TIME OBSERVATION OF THE HETEROGENEOUS RELAXATION OF A GLASS

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Understanding the physics of glass formation and devitrification remains a major challenge despite more than a century of experimental and theoretical research. This difficulty stems from the contrast between the subtle structural changes at the glass transition and the dramatic variations in dynamics that accompany them, often attributed to the emergence of spatio-temporal dynamic heterogeneities characterized by a growing correlation length. Experimental investigation of these phenomena is hindered by the limited ability to access deeply supercooled yet equilibrated states.

Ultrastable glasses, which are equivalent to ordinary glasses equilibrated far down the energy landscape and are inaccessible through conventional cooling or aging protocols, offer a promising route to overcome this limitation. Here, we exploit this approach to produce glasses with tunable kinetic stability, from ordinary to ultrastable, and investigate their transformation mechanisms using fast scanning nanocalorimetry and atomic force microscopy.

We show that when the dominant role of the free surface in thin films is suppressed, bulk glass transformation proceeds via a nucleation-and-growth-like mechanism. Spatially distinct regions transform toward the liquid state while others remain glassy, providing direct evidence of dynamic heterogeneity. We propose a unified interpretation based on dynamic contrast between regions with different relaxation kinetics, arising from either interfacial effects or intrinsic bulk heterogeneity, and argue that this framework also applies to liquid-cooled glasses.

TEMPERATURE-DEPENDENT RELAXATION PATHWAYS IN A $GeSe_2$ GLASS: AN XPCS STUDY

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Glass dynamics shows specific effects when the glass is irradiated with intense X-ray beams. Defects arising from X-ray absorption drive atomic rearrangements and induce a measurable dynamics [1,2]. At sufficiently low temperatures this evolution rejuvenates the glass, which eventually reaches a well-defined, unique stationary state in structure, dynamics and thermodynamics [3]. However, once temperature activates the structural relaxation pathway, it is no longer clear whether such stationary state persists: the way in which these irradiation-driven processes interact with the underlying structural mobility is not understood yet.

We probe this interplay in the chalcogenide glass $GeSe_2$ using X-ray Photon Correlation Spectroscopy (XPCS) across a wide temperature range. Far below T_g, the dynamics is indeed fully beam-induced; near and above T_g, it coincides with the expected α-relaxation. In between these limits, the coupled action of temperature and X-ray dose reshapes the evolving defect population, preventing the system from settling into a clear stationary regime. The competing tendencies to rejuvenate and anneal the glass generate non-equilibrium states inaccessible by thermal processing alone. This highlights both the need of new models of beam-induced dynamics and the potential of controlled irradiation to explore and manipulate the configurational landscape of glasses, together with the possibility of tuning their properties through irradiation.

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X-RAY DRIVEN AMORPHOUS-AMORPHOUS TRANSITIONS IN V-GeO_2

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We show that intense X-ray irradiation provides a non-thermal route to drive amorphous–amorphous transitions in vitreous GeO_2. By combining X-ray Photon Correlation Spectroscopy, X-ray diffraction, and Inelastic X-ray Scattering, we probe in real time the structural and dynamical response of the glass under strong irradiation.

Under high radiation doses, $\mathrm{v}-\mathrm{GeO}_2$ enters a stationary flowing regime with relaxation times of a few seconds, weakly temperature-dependent below T_g. Diffraction reveals a broadening and shift of the first sharp diffraction peak and an increase of the low-Q intensity, indicating enhanced disorder, densification, and amplified density fluctuations. These changes show a strong irradiation-temperature dependence and cannot be explained by thermal annealing.

Analysis of frozen-in and dynamical compressibility contributions indicates that the irradiated glass behaves as if quenched from a high fictive temperature, reaching values of order 1.5 T_g at room temperature. These results demonstrate a clear X-ray–driven transition toward a rejuvenated amorphous statethat is hardly accessible by conventional melt-quenching methods.

THE MATERIAL TIME OF PHYSICAL AGING – AND BEYOND

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All glassy materials undergo physical aging, that is the slow evolution of material properties as the system approaches an equilibrium supercooled liquid state. Physical aging is non-linear in temperature history, meaning that the relaxation pathway depends critically on its temperature history. In 1971, Narayanaswamy proposed that aging becomes linear when described in terms of *material time* rather than standard time. It can be viewed as a material's inner clock whose rate changes as the material ages [1,2]. This idea implies that physical aging is governed by the same mechanisms as equilibrium structural relaxation—but with a time-dependent relaxation rate.

We show how material time can be determined experimentally from time-resolved autocorrelation functions obtained by light scattering. For different systems, we demonstrate that the extracted material time renders physical aging linear in temperature history, with stationary and time-reversible thermal fluctuations [3].

Finally, we discuss mechanisms beyond material-time scaling found in metallic glasses using time-resolved XPCS. These systems exhibit compressed-exponential relaxation, whose appearance correlates with off-equilibrium values of the material's density. While the microscopic dynamics do not obey material-time scaling, the evolution of the density shows an asymmetry of approach—as expected for aging obeying material time—suggesting the material-time formalism may still apply at a more global scale.

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MICROSCOPIC ORIGIN OF THE BOSON PEAK IN MODEL GLASSES

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The excess of vibrational states known as the boson peak is a hallmark of amorphous solids, yet its microscopic origin has long remained controversial. By analyzing vibrational spectra and phonon dynamics in two- and three-dimensional model glasses with isotropic [1–3] and frustrated spin interactions [1,4], we identify a resonance-driven mechanism underlying this anomaly. We show that acoustic phonons hybridize strongly with a distinct band of intrinsic nonphononic vibrational modes when their frequencies coincide, giving rise to both the boson-peak excess in the vibrational density of states and pronounced anomalies in phonon propagation. Two classes of vibrational defects play complementary roles: low-frequency quadrupolar quasi-localized modes, which govern nonaffine mechanical responses, primarily contribute to Rayleigh scattering of phonons, whereas higher-frequency string-like modes couple resonantly to phonons and dominate the boson-peak regime. Together, these results establish phonon–string resonance as the fundamental microscopic origin of the boson peak and provide a unified defect-based framework for understanding vibrational anomalies in amorphous materials.

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THE INFLUENCE OF FROZEN-IN STRESSES ON THE VIBRATIONAL EXCITATIONS IN GLASSES

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We address the impact of frozen-in stresses in addition to spatially fluctuating elastic constants on the vibrational excitations in glasses.

We consider the continuum limit of the dynamical (Hessian) matrix of a material, whose potential energy is composed of pairwise potentials. This continuum harmonic energy density features terms involving spatially varying elastic constants and spatially varying frozen-in stresses. The dynamical variables are not only the local strain tensor but also the local vorticity tensor, which is the asymmetric counterpart of the strain. From our newly derived elastic energy density of a glass [1] we derive equations of motion of a generalized elasticity theory, which includes the role of frozen-in stresses. The stresses are intimately coupled to the local vorticities, and the statistics of the stresses governs the vibrational spectrum of the vorticity-related non-phononic excitations of the glass. As shown more than 25 years ago by S. Alexander, the local internal stresses play a vital role in the vibrational dynamics of amorphous solids, and become dominant in soft and granular matter.

We call the stress-induced excitations Type-II non-phononic excitations in contrast to the heterogeneous-elasticity-induced Type-I non-phononic excitations, which give rise to the boson peak. The Type-II excitations share many features of "quasi-localized vibrations" postulated by Schober and Oligschleger [2] to exist in the low-frequency regime of glasses.

By means of simulations of small systems [1] we show that both types of non-phononic excitations are delocalized.

Because the statistics of the small stresses is sensitively dependent on the smooth-cutoff procedure (tapering) in computer-glass models, this may give rise to artifacts in simulational investigations. This is demonstrated by numerical simulations of small systems with varying the tapering.

We show that the anomalous low-temperature specific heat capacity of glasses may be explained in terms of the frozen-in stresses and the corresponding Type-II excitations [3].

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SUBSTITUTION-DRIVEN GLASSY ANOMALIES IN BENZENE DERIVATIVES: THE ROLE OF METHYL AND CHLORINE ARRANGEMENT

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We present comprehensive heat-capacity measurements for a series of benzene derivatives differing in both the number and spatial arrangement of chlorine and methyl substituents. The objective of this work is to identify how specific substitution patterns influence the emergence of glassy behavior in quasiplanar molecular crystals.

All studied compounds display characteristic glassy anomalies, including a linear contribution to the heat capacity associated with two-level systems and either smeared or broad maximum near 10 K in the C_p/T^3 vs T representation, consistent with the presence of a boson peak.

By examining molecules that vary subtly in their substitution motifs — such as symmetric versus asymmetric placement of methyl groups, or differing chlorine–methyl arrangements — we identify trends in the magnitude and position of the boson peak. Our results show that the density of two-level systems is governed not only by the number of methyl substituents but also by their precise positions. In particular, equally or inversely substituted configurations highlight how small changes in molecular geometry can significantly modify the low-energy excitation landscape. This demonstrates that molecular asymmetry plays a more decisive role than the overall degree of orientational disorder in shaping the glassy response.

These findings are discussed in the context of current theoretical models and prior experimental observations, offering new insight into how substitution-driven structural motifs control glassy anomalies in molecular crystals.

THE VIBRATIONAL SPECTRUM OF SILICA: HIDDEN COUNTING RULES AND MICROSTRUCTURAL DETERMINANTS

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Our understanding of vibrations in solids rests today on concepts and techniques designed for crystals, that explicitly rely on periodicity and are hence inapplicable to amorphous materials. There is no established way to decompose the vibrational spectrum of amorphous solids into the contributions of well-identified types of atomic motion, which obscures the interpretation of various experimental data accessing linear response, from vibrational to optical properties. Here, we construct such a framework for the archetypal covalent glass – silica – by repeated use of the projection formalism. Applying the projection formalism iteratively permits one to split the vibrational spectrum of silica into weakly coupled eigenspaces organized into a hierarchical structure. These groups, separately, and their partial hybridization are shown to account for major features of the spectrum.

HIGH-FREQUENCY SOUND ATTENUATION OF VITREOUS SILICA PROBED BY EXTREME UV TRANSIENT GRATING SPECTROSCOPY

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Glasses present a plateau in the temperature dependence of the thermal conductivity at temperatures of a few Kelvin. The plateau is a universal feature associated with Rayleigh scattering of sound between 100 GHz and 1 THz, a regime where the sound attenuation grows as the fourth power of frequency. The measurement of the sound attenuation in the relevant frequency range is particularly challenging to experiments.

Here we report on the measurement of the sound attenuation of vitreous silica membranes using the newly developed technique of extreme ultraviolet transient grating. The setup exploits the extreme UV pulses of the Fermi free electron laser (FEL) in Trieste to perform transient grating spectroscopy. Two pump beams overlap on the sample and generate a transient intensity grating that induces the generation of a phonon of a well-defined wavelength. A third beam is delayed with respect to the pump beams by means of a delay line and used as a probe. The detected signal gives information on both the phonon propagation and damping, combined with the thermal diffusivity at the probed wavevector. In this way, it is possible to measure sound velocity, sound attenuation and thermal diffusivities of thin films and membranes up to $\sim$ 400 GHz. We measured the sound attenuation at three different frequencies and at two temperatures, 50 K and room temperature.

The measured data are compared with those obtained with other methods in a wide frequency and temperature range. Sound damping in silica can be modeled by a combination of Rayleigh-like scattering and anharmonic and relaxational mechanisms. A main result is that the purely anharmonic processes involved in sound attenuation have the same dependence on frequency and temperature both in crystals and glasses.

CONTINUOUS PHASE TRANSITIONS IN ACTIVE PARTICLES MATTER

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I will review some recent results regarding continuous phase transition in active particles systems. In the first part of the I will focus on simulations of active particles interacting via a quorum-sensing (QS) mechanism by which particles change their swimming speed based on the number of perceived neighbors. I will show that if these particles slow down enough when interacting, the system undergoes a full motility-induced separation (MIPS) and that the coexistence curve terminates into a critical point belonging to the Ising universality class [1]. In contrast I will also show recent results demonstrating that, if these QS interactions have two competing scales, the MIPS is destabilized and the system forms an active micro-emulsion which is well described by a renormalized field-theory in a effective equilibrium framework. Finally I will discuss some recent experiments in which super-paramagnetic colloids activated by a bath of swimming E. coli undergo two-dimensional melting out of equilibrium [2]. I will show how the basic physics of the experimental active crystal is well reproduced by a schematic model of active particles and how the KTHNY-theory remains qualitatively valid in describing the melting scenario of this active solid.

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ARTIFICIAL LIFE OF AN ACTIVE DROPLETS SYSTEM: A QUANTITATIVE LIFECYCLE ANALYSIS

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The study of synthetic active matter systems holds the promise for designing smart materials and devices with emergent characteristics akin to those of living organisms, eventually opening the doors to the realization of artificial life. Such an investigation, however, is challenged by the difficulty inherent in identifying the relationship between the features of the elementary constituents and the emergent properties of the whole; to this end, a key step consists in the accurate quantification of the system's observed behavior. Here, we report the study of a small ensemble of confined self-propelled oil droplets floating on the surface of an aqueous solution, comprising equal numbers of red- and blue-stained agents: the colorants affect the droplets' interfacial tension properties differently, consequently influencing their collective dynamics. Droplet trajectories extending for up to 5 hours are extracted from video recordings with a tracking pipeline developed ad hoc. The structural and dynamical analysis of the system reveals a "life-to-death" cycle unfolding in qualitatively distinct stages, showcasing a complex interplay between individual droplet mobility and collective organization. The tools developed and the results obtained in our work pave the way for the *in silico* modeling as well as the experimental design of synthetic active matter systems displaying life-like and programmable behavior.

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Symmetry-breaking processes drive multicellular rosette morphogenesis

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Multicellular rosettes are observed in different situations such as morphogenesis, wound healing, and cancer progression. While some molecular insights have been gained to explain the presence of these assemblies of five or more cells around a common center, what are the tunable, global features that favors/hinders their formation is still largely unknown [1]. Here, we made use of a Voronoi dynamical model [2] to investigate the ingredients driving the emergence of rosettes characterized by different degree of stability and organization. We found that (i) breaking the local spatial symmetry of the system, i.e., introducing curvature-inducing defects, allows for the formation of rosette-like structures (ii) whose probability of formation depends on the characteristic of the cellular layer. In particular, a trade-off between tissue fluidity and single cell deformability dictates the assembly of transient rosettes, that are strongly stabilized in the presence of cell alignment interactions [3]. Overall, our work may set the stage to gain an unifying understanding of the plethora of biophysical mechanisms involving the occurrence of rosette-like structure both in physiology and their altered formation in pathology.

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Soft modes in vector spin glass models on sparse random graphs

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In Ref. [1] we study numerically the Hessian of low-lying minima of vector spin glass models defined on random regular graphs. We consider the two-component (XY) and three-component (Heisenberg) spin glasses at zero temperature, subjected to the action of a randomly oriented external field. Varying the intensity of the external field, these models undergo a zero temperature phase transition from a paramagnet at high field to a spin glass at low field. We study how the spectral properties of the Hessian depend on the magnetic field. In particular, we study the shape of the spectrum at low frequency and the localization properties of low-energy eigenvectors across the transition. We find that in both phases the edge of the spectral density behaves as $\lambda^{3/2}$: such a behavior rules out the presence of a diverging spin-glass susceptibility $\chi_{\text{SG}} = \langle 1/\lambda^2 \rangle$. As to low-energy eigenvectors, we find that the softest eigenmodes are always localized in both phases of the two models. However, by studying in detail the geometry of low-energy eigenmodes across different energy scales close to the lower edge of the spectrum, we find a different behavior for the two models at the transition: in the XY case, low-energy modes are typically localized; in the Heisenberg case low-energy eigenmodes present a multi-modal structure (a sort of "delocalization"). These geometrically non-trivial excitations, which we call Concentrated and Delocalized Low-Energy Modes (CDLEM), coexist with trivially localized excitations: we interpret their existence as a sign of critical behavior related to the onset of the spin glass phase.

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MULTIPHOTON QUANTUM SIMULATION OF A GENERALIZED DENSE HOPFIELD NEURAL NETWORK

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We introduce, develop, and investigate a connection between photonic quantum interference, a core element of emerging photonic quantum technologies, and dense multi-synaptic Hopfield neural networks for associative memory [1]. Specifically, we show that combining a system composed of $N_{\rm ph}$ indistinguishable photons in superposition over M field modes, a controlled array of M binary phase-shifters, and a linear-optical interferometer, yields output photon statistics described by means of a $p = 2N_{\rm ph}$-synaptic Hopfield Hamiltonian of M Ising-like neurons ±1. The role of *memories*, in the statistical physics context, is played by the permanents of the scattering matrix of the interferometer. As an exemplification of such a mapping, we numerically investigate the generalized 4-body Hopfield model (2 photon states), undergoing a transition from a memory retrieval to a memory black-out regime, i.e., a spin-glass phase, as the amount of stored memories increases. As the noise in the neural network increases, the system undergoes a phase transition to a paramagnetic phase. The mapping enables novel routes to the realization and investigation of disordered complex classical systems via efficient photonic quantum simulators and describes aspects of structured photonic systems in terms of classical spin Hamiltonians.

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On the role of molecular details in structural relaxation

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The traditional picture of structural relaxation implies that at high temperatures all molecules in a system perform rotational diffusion with a single relaxation time, leading to a monoexponential rotational correlation function. Upon lowering the temperature, the dynamics is thought to become heterogeneous, leading to a distribution of relaxation times and a corresponding stretching of the correlation function. However, this simple picture is generally not supported by observations, since, in many cases, relaxation stretching, the extent of which differs between liquids, is still present at temperatures far above the melting point and even obeys time-temperature superposition in a certain temperature range [1,2]. Furthermore, it was shown recently that the self part of the rotational correlation function close to the glass transition temperature shows a generic shape [3], suggesting a peculiar transition from a high- to a low temperature behaviour, rather than a continuous broadening. In this talk, we give a quick overview of literature results challenging the common interpretation of the relaxation shape and then present recent results from combined dielectric spectroscopy, light scattering, NMR and MD simulation studies, demonstrating that anisotropic rotations and internal molecular flexibility substantially contribute to structural relaxation in the liquid state, leading to diverse relaxation shapes. However, molecular individuality diminishes upon approaching the supercooled-liquid regime, revealing the generic character of structural relaxation.

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LINEAR LOW-TEMPERATURE HEAT CAPACITY IN GRAPHITE-DERIVED NANOSTRUCTURES

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Low-temperature heat capacity provides a sensitive probe of low-energy excitations in carbon-based solids, where reduced dimensionality, disorder, and electronic effects compete. In this report, we present a comparative study of the specific heat of several graphite-derived materials — multi-walled carbon nanotubes (MWNTs) [1], exfoliated graphite [2], and graphene oxide [3] — measured in the temperature range where deviations from the conventional Debye T^3 law become pronounced. All investigated systems exhibit a clear linear term in the heat capacity at low temperatures, $C(T) = \gamma T + \beta T^3 + \ldots$, whose magnitude and physical origin strongly depend on the material structure. For MWNTs, the linear contribution is consistent with quasi-one-dimensional phonon modes and, in metallic tubes, an additional electronic component. In exfoliated graphite, the linear term reflects the combined effect of strong structural anisotropy, interlayer decoupling, and low-energy out-of-plane vibrational modes characteristic of weakly coupled graphene layers. In graphene oxide, the linear term is significantly enhanced and is attributed to disorder-induced low-energy excitations, including localized vibrational states and defect-related two-level systems.

The comparative analysis highlights the non-universal nature of the linear heat-capacity term in graphite materials and demonstrates its sensitivity to dimensionality, interlayer interactions, and defect structure. These results emphasize the importance of low-temperature calorimetry for disentangling phononic, electronic, and disorder-related contributions in carbon-based materials and for understanding their thermodynamic behavior beyond the Debye model.

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DYNAMICS OF VISCOUS LIQUIDS AND THE RANDOM BARRIER MODEL

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Despite its simplicity, the Random Barrier Model (RBM) has been found to describe the ac conductivity of many glasses [1] and ioniq liquids [2] surprisingly well. The RBM has been solved analytically in the sense that a good understanding of the physics governing the model is at hand, leading to a very accurate description of the universal ac conductivity [3].

An unresolved mystery is why the RBM also describes very well the frequency dependent fluidity (inverse of shear viscosity) of many non-ionic liquids [2], as well as the mean-square displacement of model glass-formers [4,5]: The RBM considers non-interacting particles jumping stochastically on a simple cubic lattice with identical site energies and random energy barriers for nearest-neighbor jumps – i.e., far from how we usually think about a viscous liquid. Utilizing new results from extensive computer simulations [5], the present contribution investigates this mystery.

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Competing Length Scales and Screening in Dense Electrolytes

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Understanding electrostatic screening in concentrated electrolytes remains a central challenge, particularly in light of experiments reporting screening lengths that grow anomalously with salt concentration. Using extensive molecular dynamics simulations of a prototypical non-aqueous electrolyte, $LiBF_4$ dissolved in ethylene carbonate, we investigate structural, dielectric, and transport properties over a concentration range spanning the dilute Debye–Hückel regime to solvent-in-salt conditions. We show that conventional screening lengths, associated with charge–charge correlations and renormalized ionic charges, decrease with concentration and display only regular underscreening on nanometric scales. In contrast, the system undergoes a progressive formation and growth of extended ionic clusters that eventually percolate into a gel-like network. We identify the characteristic size of these ionic domains as a second, independent length scale that increases strongly with concentration. By comparing these two competing lengths, we demonstrate that the experimentally observed anomalously large screening lengths are more naturally interpreted as reflecting the spatial extent of growing ionic domains rather than the range of pairwise electrostatic interactions. This unified picture reconciles simulations and experiments and clarifies the physical origin of anomalous underscreening in dense electrolytes.

WHICH PROCESSES DEFINE THE PROPAGATION OF COLLECTIVE EXCITATIONS IN SIMPLE AND BINARY LIQUIDS?

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Analysis of collective dynamics in liquids from scattering experiments or computer simulations is usually based on application of a second-order memory function Ansatz, which assumes several channels of correlation decay in the highest memory function. However, such an approach allows one to recover experimental/simulated dynamic structure factors but does not shed light on the processes responsible for the mechanism of propagation of collective excitations. Traditional phonons known from the solid state theory do not exist in liquids, therefore it is important to have a methodology which enables estimation of the leading processes contributing to the propagation of collective excitations in liquids. In particular, for the case of one-component liquids it is important to estimate how the origin of acoustic modes is changing with increasing wave numbers from macroscopic viscous to atomic-scale elastic regime. For many-component liquids another issue is important: there are several types of collective excitations (acoustic and optic-like), dispersion laws of which depend on the mass ratio of components.

We will report a method of analysis of eigenvectors associated with dynamic eigenmodes in several simple and binary Lennard-Jones liquids. The dynamic eigenmodes are obtained as solutions of the generalized Langevin equation in matrix form. Our analysis reveals different origin for macroscopic and short-wavelength acoustic modes in liquids and how it changes with the increase of wave numbers. For binary liquids the origin of high- and low-frequency excitations will be discussed.

When liquids flow on solids: unexpected deep liquid-solid coupling

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A liquid flows on a solid surface, do we expect that the liquid in motion modifies the phonon dynamics of the solid substrate? We present new experiments carried out at room temperature showing a strong liquid/solid dynamic interdependence. This interdependence is highlighted using high resolution inelastic methods, studying the THz dynamics of an Alumina monocrystal, in the dry state and when a thin layer of water flows on it. Alumina was chosen because of its high wetting power (high energy surface). We show that dramatic changes occur in the vibrational state of the Alumina affecting both transverse and longitudinal acoustic phonons during contact wit liquid water [1]. The induced effects on solid are reproducible, reversible and extended deep in the crystal ($> 250\ \mu$m) excluding a confined nanosurface effect [2]. Therefore, a solid wall can no more be considered as only a simple means to confine and limit the propagation of a fluid, but that it is in turn also a dynamically "deformable" medium via a phononic long-range coupling whose impact only begins to be identified. These new results suggest the existence of long range coupling in agreement with new insights about liquids predicting that solid-like stresses propagate in confined liquid [3,4].

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POLARIZATION DYNAMICS

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Understanding the fluid dynamical properties on the nano-scale gives fundamental new insight into the underlying processes in fluids. In this talk, a dynamical equation for polarization is derived from the microscopic definition of the molecular dipoles revealing the presence of a diffusive process which couples the polarization to the molecular mechanics. Through molecular dynamics simulations of water it is shown that the dispersion relation for the dielectric spectrum is proportional to the wave-vector squared confirming the diffusive process. The dynamical equation is applied to different scenarios, where the characteristic length scale is on the order of a few nanometers; it is shown that the diffusion process can significantly reduce the dielectric response of any dielectric material on these length scales.

UNIFIED THEORY OF PHONON IN SOLIDS WITH PHASE DIAGRAM OF NON-DEBYE ANOMALIES

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The classical Debye model successfully predicts the phononic contribution to the specific heat of solids in the continuum limit. However, as the phonon wavenumber increases, their vibrational density of states gradually deviates from the Debye prediction and eventually manifests as the Van Hove singularities for crystals, and a boson peak for glasses. To date, there is still much controversy over whether these two non-Debye anomalies are equivalent or not. Here, we propose a unified model and demonstrate that it describes the vibrational density of states in both crystals and glasses. We achieve this by treating the vibrational excitation of solids as the elastic phonons resonating with local modes. Our modeling enables the construction of a phase diagram of non-Debye phonon anomalies. We clarify that the Van Hove singularity and boson peak can evolve as two variants of the same entity when the dispersion displays continuous softening; otherwise, they emerge separately due to resonance-induced extra acoustic softening, further proved by their coexistence. The model is supported by a comparison with experimental heat capacity data over a wide range of real solids, including 143 crystalline and glassy substances. These findings provide a unified picture of the Van Hove singularity and boson peak, and deepen our fundamental understanding of continuum elasticity of real solids.

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ON THE EUCLIDEAN RANDOM MATRIX MODEL OF VIBRATIONS IN GLASS

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Understanding the mechanical and vibrational properties of disordered solids remains a central challenge in glass physics. The Euclidean random matrix (ERM) model provides a minimal yet comprehensive framework by representing particles as performing small displacements around random positions within a harmonic approximation. It captures both long-wavelength sound modes and disorder-induced random-matrix excitations, offering insight into vibrational anomalies such as the boson peak and the damping of acoustic waves.

We present numerical data and a self-consistent theoretical analysis that identifies an elastic instability, viz. a critical point where increasing disorder destabilizes the ERM network of harmonic interactions [1]. As the coordination number decreases, the mechanical response softens, and floppy modes emerge below the transition. At the transition, the shear modulus vanishes continuously, and the vibrational density of states develops a low-frequency plateau extending to zero.

Our results establish the ERM model as a paradigmatic theoretical tool for studying the universal vibrational and mechanical anomalies of glasses and highlight the fundamental connections between non-affine elasticity, sound damping, and marginal stability near the jamming transition.

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UNVEILING GLASS-LIKE BEHAVIOR IN MOLECULAR CRYSTALS WITH MINIMAL DISORDER: THE KEY ROLE OF ANHARMONIC VIBRATIONS IN P-CHLORONITROBENZENE

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The low-temperature heat capacity of p-chloronitrobenzene (p-CNB) has been measured for the low-temperature fully ordered phase II and the high-temperature orientationally disordered phase I. Phase II apparently behaves as a typical Debye solid. Phase I, with minimal disorder arising from two possible molecular orientations within a monoclinic lattice, can be supercooled to nearly 0 K and low-temperature glassy anomalies emerge. Phase I exhibits tunneling two-level systems (TLS) but lacks any signature of a Boson Peak (BP), with a Debye level about four times higher than that of the ordered phase II, indicating a softening of the acoustic phonons in the disordered phase I. Specific heat data were rationalized by measurements of the vibrational density of states (VDOS) obtained from inelastic neutron scattering experiments. They reveal a shift of the vibrational modes towards lower energies in phase I compared to phase II, within the same energy range.

Ab initio molecular dynamics simulations (only when explicitly including anharmonicity) reproduce notably well the experimental VDOS of both phases providing a consistent microscopic description of the vibrational dynamics. Thus, anharmonic effects do not necessarily lead to an excess over the Debye level (a BP-like anomaly), as even the fully ordered phase II also exhibits strong anharmonicity despite showing Debye-like behavior in both the experimental VDOS and heat capacity data.

DECOUPLING DENSITY AND DISORDER EFFECTS ON THE BOSON PEAK IN METAL-ORGANIC FRAMEWORKS

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The boson peak is a vibrational feature observed as an excess of vibrational modes beyond the level expected by the Debye model. This has been showcased in many crystalline and glassy structures of very varying compositions, but its origin is still unclear. Both theoretical and experimental studies suggest that its origin stems from structural disorder, differences in density, and local variations in elasticity, amongst others. However, in most cases, the tested amorphous or glassy polymorphs are less dense than the corresponding crystals, i.e., both density and disorder affect the boson peak intensity and position in a similar manner. To overcome this, we have used inelastic neutron (ISIS) and X-ray scattering (ESRF) to test the boson peak in a metal-organic framework (MOF) system of composition Zn(Imidazolate)2, as polymorphs with varying density and disorder exist. This includes a very porous and crystalline structure (ZIF-4), which upon heat treatment, first collapses into a high-density amorphous phase (ZIF-HDA) before crystallizing into a structure denser than ZIF-4 (ZIF-zni). Further heating leads to melting and glass formation upon cooling (ZIF-glass). By probing the different polymorphs, we showcase how the boson peak is inherently bound to structural disorder. Our results provide new insights into the nature of boson peak and its correlation with fundamental structural parameters.

EMERGENT GLASS-LIKE DYNAMICS AND LOW-ENERGY EXCITATIONS IN CESIUM HALIDE PEROVSKITES: A VIBRATIONAL PERSPECTIVE ON STRUCTURAL COMPLEXITY

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Crystalline perovskites have emerged as an unexpected platform for glass-like thermal behaviour, challenging the typical distinction between ordered and disordered solids. We explore glassy anomalies in Cesium Halide Perovskites (CsHPs) of different dimensionality and chemical complexity, including 3D single ($CsPbBr_3$) and double perovskites ($Cs_2AgBiBr_6$) and a 0D (Cs_4PbBr_6) phase. By combining Raman spectroscopy, specific heat, and thermal conductivity measurements ($2 - 300$ K), we uncover an excess of vibrational states below 100 cm^{-1} analogous to the boson peak observed in glasses and arising from phonon localization, mode softening, and dynamic disorder. The low energy excess correlates with a dimensionality-controlled evolution from an extended phonon-mediated propagation in the 3D network to markedly localized vibrations in the 0D compound, where thermal transport acquires a glass-like character. The emerging picture points to a progressive breakdown of the phonon-gas model with two key implications: (i) CsHPs offer a chemically tunable setting to probe the transition from phonon-mediated (crystalline) to diffusion/locon-dominated (glassy) heat conduction; (ii) elucidating this crossover provides design principles for intrinsically phonon-glass electron-crystal systems that do not rely on extrinsic disorder. Overall, these findings establish CsHPs as a model system to explore universal thermal anomalies and incipient glassy dynamics in soft crystalline lattices.

PHOTON CORRELATION METHODS AT THE MID INSTRUMENT AT EUROPEAN XFEL

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The European X-ray Free Electron Laser (EuXFEL) delivers ultra-short, highly coherent hard X-ray pulses at megahertz repetition rates, enabling unique coherent scattering and imaging experiments. This talk introduces the Materials Imaging and Dynamics (MID) instrument at EuXFEL [1] and highlights different experimental campaigns that exploit these beam properties and the available instrumentation. A key technique at MID is X-ray Photon Correlation Spectroscopy (XPCS) at MHz repetition rates, which enables access to nanometer length scales and sub-microsecond dynamics in small-angle scattering (SAXS) geometry. This spatio-temporal range is ideally suited to study diffusion processes in dense environments, as well as early-stage aggregation and phase transitions in soft-matter systems. We present the hard- and software implementations that establish a user-facing experimental pipeline available as a standard configuration at MID (SAXS-XPCS) [2]. Representative applications include aggregation of antibody proteins [3], temperature-jump phase transitions in stimuli-responsive polymers [4], molecular crowding effects in dense protein solutions [5,6], anomalous transport and cage dynamics in crowded egg yolk-plasma environments [7], as well as container-less MHz-XPCS using an acoustic levitation sample environment [8]. Beyond this standard configuration, further developments are introduced that aim to extend the accessible time and length scales (towards faster dynamics and smaller real-space features). Additionally, we demonstrate the application of X-ray Cross-Correlation Analysis (XCCA). Crystallization, one of the most fundamental phase transitions, is in many respects challenging to study in atomic and molecular liquids because of the spontaneous nature of the process and the very short timescales and small lengthscales involved. By combining micrometer-wide liquid jets that rapidly supercool and crystallize upon injection into vacuum with femtosecond X-ray scattering, we probe early-stage crystallization while overcoming ensemble averages inherent to conventional X-ray scattering. This serial diffraction approach provides a stringent test of classical nucleation theory in noble-gas liquids (Krypton and Argon) [9] and opens the possibility to quantify deviations from ideal crystal structures, such as stacking faults and twinning, via XCCA [10].

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DEVELOPMENT OF HETERODYNE BRILLOUIN MICROSCOPY

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Mechanical properties play a fundamental role in regulating biological processes, and their alteration is a hallmark of disease, including neurodegenerative disorders. Brillouin microscopy has emerged as a key non-contact technique for probing viscoelasticity with sub-micron resolution. While state-of-the-art implementations rely on complex dispersive spectrometers, this work investigates heterodyne detection as an alternative paradigm to enhance the accessibility of the technique.

We present the development and systematic evaluation of a heterodyne Brillouin microscopy setup. The study focuses on the physical principles of detection, providing a comprehensive noise analysis and signal-to-noise ratio modeling. The performance of the heterodyne approach is quantitatively compared against conventional spectrometer-based detection using benchmark measurements.

Results reveal that while heterodyne microscopy offers significant flexibility in spectral resolution, its sensitivity is effectively limited by the intrinsic manner in which signal and noise are jointly integrated within the detection bandwidth. This work defines the fundamental performance boundaries of the technique, clarifying the trade-offs between flexibility and sensitivity, and provides critical insight into the domain of applicability for heterodyne schemes in quantitative biomechanical imaging.

SETUP COMBINING FAST SCANNING CALORIMETRY WITH X-RAY TOTAL SCATTERING

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We introduce an experimental setup that combines fast scanning calorimetry and X-ray total scattering, enabling real-time measurements of nanoscale structural changes in our samples during and after rapid temperature scans [1]. The core of the system is a vacuum chamber that allows diffraction measurements with a high signal-to-background ratio even for amorphous materials, making it possible to resolve subtle structural differences between sample states. While demonstrated at beamline ID15A of the ESRF, the setup is portable and can be implemented at other synchrotron beamlines as well. This presentation includes details of the system's design and showcases several examples of its early applications, including one that takes advantage of high cooling rates up to 10^4 K/s. Our approach opens up new opportunities for studying the interplay between structure and thermodynamics in complex materials.

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A phase-field model for solutions of DNA-made particles

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Understanding how microscopic interaction rules generate emergent mesoscale organization is a central problem in complex systems and soft matter. In this talk, I present a continuum phase-field description of liquid-liquid phase separation in solutions of DNA nanostars, a model system of programmable, limited-valence building blocks. Starting from a coarse-grained free-energy functional, we derive and numerically solve a Cahn-Hilliard model that captures both equilibrium phase behavior and nonequilibrium coarsening dynamics. The approach semi-quantitatively reproduces experimentally observed phase boundaries and links microscopic interaction parameters to macroscopic pattern formation [1].

I then show how the same framework can be extended to multicomponent condensates stabilized by heterogeneous, specific interactions, focusing on immune-induced antibody-DNA hybrid condensates. In this case, the phase-field model captures concentration-dependent condensation, reversibility, and orthogonality across multiple antibody-antigen pairs [2]. Overall, this work highlights phase-field modelling as a useful framework to connect molecular programmability with emergent collective behavior in phase-separating DNA-based systems.

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A MINIMAL MOLECULAR MODEL FOR PROBING THE ROLE OF RNA IN PROTEIN CONDENSATES

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Liquid–liquid phase separation (LLPS) underlies the formation of membraneless organelles that regulate cellular processes in physiological and pathological contexts [1]. Protein phase separation has been predominantly associated with intrinsically disordered regions (IDRs) and low-complexity sequences, but the minimal sequence determinants and building blocks underlying LLPS remain incompletely understood.

Here, we investigate all combinations of minimal peptides to assess their propensity to undergo phase separation using atomistic molecular dynamics simulations.To mimic aspects of crowded cellular conditions [2], simulations are performed at high peptide concentrations. Crucially, to capture key features of biomolecular condensates, we introduce nucleic acids, modeling RNA-enriched environments and probing their impact on peptide self-association.

We find that several dipeptides rapidly form clusters, demonstrating that even minimal peptide units encode sufficient multivalency to promote LLPS. These results suggest that LLPS is a general property of peptides and proteins, not exclusively dependent on IDRs or long sequence length. By analyzing cluster fluidity and local structural order, we further distinguish between liquid-like and dynamically arrested solid-like assemblies. In several cases, clusters exhibit glass-like behavior, indicating that arrested condensates may represent long-lived states rather than merely late-stage transitions from liquid to solid phases.

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POLYCATENANE ASSEMBLY WITH TOPOII IN TOROIDAL CONFINEMENT

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Poly-catenanes - chains of mechanically interlinked molecular rings - represent an emerging class of topological materials with fine-tunable properties. Linear polycatenanes generalize the property of polymers, while previous computational results [1] have shown that circular polycatenanes generalize dsDNA plasmids, including plectoneme formation induced by supercoiling. However, their controlled synthesis remains difficult to achieve, as it requires strategies to overcome entropic barriers to obtain ring threading and closure and to design architectures with well-defined properties. This presentation focuses on a possible strategy to synthesize circular catenanes. Starting from unlinked DNA rings – such as readily available plasmids – the topology of the system is altered through the action of the topoisomerase II (TopoII), an enzyme which modifies DNA topology by cutting and joining pairs of double-strands. We employed a geometric confinement to enhance catenation by forcing the rings along a circular path. A range of confinement regimes has been systematically explored to investigate how geometry affects the behavior of polymers and the formation of interlocked structures. Our analysis shows that in the Odijk regime, the system evolves into a variety of linked yet unknotted structures, providing a possible pathway toward catenane formation.

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A MICROFLUIDIC DEVICE FOR SINGLE-CELL ANALYSIS OF T-CELL GROWTH AND PROLIFERATION

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We develop a novel microfluidic device designed to track the proliferation of single mammalian cells via live-cell microscopy.

While numerous systems exist for single-cell proliferation studies, most are optimized for bacteria. We present a device specifically designed for human T cells, featuring an array of microchannels that trap single cells without altering their physiological growth conditions. Each channel allows one cell to enter and proliferate under a constant flow of nutrients, enabling long-term tracking over multiple generations while preserving cell viability.

The device geometry ensures stable trapping and allows continuous observation of cell growth, division, and progression through the phases of the cell cycle. Through time-lapse microscopy, individual cells can be identified and quantitatively analyzed, measuring key parameters such as cell size dynamics, duplication time, and cell-cycle-dependent growth behavior.

We validated the device by reproducing and extending previous findings on human Jurkat T cells, confirming their symmetric volume division. We use it to follow the growth and division of human primary T cells at single cell level by measuring:(i) duplication time, assessing the effect of growth in isolation; (ii) cell size dynamics, from birth to mitosis, to determine their growth mechanisms. Overall, our device design can be easily adaptable and can be used to study different cell types and sizes while maintaining the same high trapping efficiency.

COHERENT X-RAY SCATTERING OF FLUCTUATIONS AND DYNAMICS IN COMPLEX SYSTEMS

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Understanding collective dynamics and structural heterogeneities in complex fluids requires experimental access to mesoscopic length scales and micro- to femtosecond time scales. In this contribution, we present two complementary studies that exploit coherent X-ray techniques to probe fluctuations and transport in biologically and physically relevant disordered systems. First, we use megahertz X-ray Photon Correlation Spectroscopy (MHz-XPCS) at an X-ray free-electron laser to directly access protein dynamics in crowded solutions on microsecond time scales. Measurements of ferritin reveal a continuous crossover from Brownian to anomalous diffusion with increasing concentration, manifested by non-exponential correlation functions and the emergence of cage effects at molecular length scales. By combining XPCS with small-angle scattering and hydrodynamic modeling, we disentangle short- and long-time diffusion regimes and quantify the role of many-body hydrodynamic and direct interactions in dense biological matter. Second, we investigate supercooled glycerol–water microdroplets using femtosecond coherent X-ray scattering to outrun crystallization and access deeply supercooled states. Enhanced small-angle scattering reveals growing density fluctuations and correlation lengths upon cooling, consistent with supercritical behavior associated with the liquid–liquid transition scenario of water. Comparison with molecular dynamics simulations shows that dilute glycerol shifts and partially suppresses these fluctuations, providing insight into how solutes modify water's anomalous thermodynamics.

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Tiny movements, big changes: when slow dynamics decides how fast liquids and glasses relax

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In simple liquids and soft materials, equilibration is typically governed by the α-modes, which control density fluctuations and whose characteristic timescales increase rapidly upon cooling. A growing body of experimental results suggests, however, the existence of an alternative equilibration pathway with a much weaker temperature dependence, characterized by a temperature-invariant activation barrier on the order of $100\,\mathrm{kJ\ mol^{-1}}$. We identify the molecular origin of this class of equilibration mechanisms with the slow Arrhenius process (SAP), detected by dielectric spectroscopy and related techniques [1–5]. The SAP is described within the collective small displacements (CSD) model, in which local amorphous packing is reorganized through molecular motions that are small in amplitude compared to those involved in the α-modes [6]. By combining this picture with a statistical-mechanics-based equation of state capturing nonbonded segmental interactions, the CSD model predicts the SAP activation energy a priori based solely on thermodynamic material properties. Finally, based on experimental findings on polymers and small molecules, we present a framework for soft material equilibration that provides quantitative predictions for technologically relevant processes, including polymer adsorption on silicon wafers [7] and crystal growth of small organic molecules in the glassy state [8].

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HIERARCHICAL DYNAMICS AND TIME-LENGTH SCALE SUPERPOSITION IN GLASSY SUSPENSIONS OF ULTRA-LOW CROSSLINKED MICROGELS

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When a colloidal system is driven in the glassy state, it often exhibits microscopic non-equilibrium dynamics that are attributed to the relaxation of internal stresses [1]. In some systems stresses can build-up spontaneously (e.g. in gels [2,3]) or they can be induced by external factors such small temperature fluctuations. The signatures of these dynamics are compressed density-density correlation functions and super-diffusive relaxations.

In this talk, I will discuss the glass transition in suspensions of ultra-low cross-linked thermosensitive PNIPAM microgels. In this system, the glass transition can be induced by swelling the microgels with temperature variations or by preparing distinct samples with increasingly large number density. Exploiting Photon Correlation Imaging and Small Angle X-Ray Scattering, I will show that the dynamical properties of suspensions prepared with these two different approaches are essentially identical, in sharp contrast with their structure, which is very different. In addition, I will show how small temperature fluctuations can strongly change the relaxation time of the microscopic dynamics when approaching the glassy state, as well as that the dynamics exhibits a peculiar transition from super-diffusive to sub-diffusive depending on the probed length-scale, a behavior that can be rationalized in terms of hierarchical relaxation mechanisms well described by a single master curve [4].

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FICKIAN YET NON-GAUSSIAN: A NEW PARADIGM FOR DIFFUSION IN GLASSY MATERIALS

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In 2009, experiments on colloidal tracers diffusing in complex biological fluids revealed a novel type of diffusion, distinct from both standard Brownian motion and anomalous diffusion [1]. Indeed, a mean square displacement increasing linearly in time (Fickian) surprisingly coexists with a non-Gaussian displacement distribution. Since then, Fickian yet non-Gaussian Diffusion (FnGD) has been observed in a wide range of molecular and soft matter systems and is generally associated with heterogeneities in the local environment. Given that glass-forming liquids are widely regarded as the epitome of dynamic heterogeneity, a natural question arises: do they also provide a paradigmatic example of FnGD? In this talk, I will discuss how FnGD challenges the conventional understanding of microscopic diffusion. I will then present results on glass-forming liquids, drawing on experiments on colloidal systems and simulations of molecular liquids [2,3]. We find that FnGD becomes increasingly pronounced upon approaching the glass transition and follows universal scaling laws, providing new insight into dynamic heterogeneities and structural relaxation. Notably, this physical picture has recently found experimental support in glassy polymer nanocomposites [4]. Finally, I will broaden the discussion beyond supercooled liquids by presenting more recent results from ongoing projects on other glassy materials, highlighting differences, similarities, and potential universal aspects of FnGD.

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COMPLEX ASSEMBLAGE OF A SIMPLE SYSTEM: BIMODALITIES OF LOCAL ORDERING IN 2D HARD DISKS

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The fundamental question of how complex structural ordering emerges from simple hard-core interactions remains a cornerstone of statistical mechanics. In this contribution, we explore counterintuitive self-organization phenomena in two-dimensional (2D) hard disks, motivated by recent findings for quasi-one-dimensional (q1D) hard disks [1]. This particular geometry is uniquely significant because it is commensurate with the bulk 2D triangular lattice at close packing, while the confinement is sufficiently strong to prevent particles from overpassing one another.

The central discovery of the present study is the emergence, upon increasing density, of bimodal probability distributions for a local structural order parameter, defined as the distance d between a disk's alternative nearest neighbors [1,2]. In the absence of attractive forces, these bimodalities reveal purely entropic structural crossovers from a disordered, "gas" state ($d \geq 2\sigma$) to a caged, "crystal" state ($d \approx \sqrt{3}\sigma$), with three intermediate states – "liquid-like", "hexatic-like" and "crystal-like" – appearing in between ($2\sigma > d > \sqrt{3}\sigma$, where σ is the hard-core diameter). These findings demonstrate that local caging driven solely by entropy acts as a universal precursor to macroscopic ordering in 2D hard-core matter.

We further examine how these local bimodalities reconcile long-standing discrepancies in the decay of pair correlation functions observed in 2D bulk and confined geometries [3,4]. By establishing a direct connection between simple hard disk models and the concept of locally favored structures, traditionally associated with complex systems [5], our results provide a refined theoretical framework for understanding self-assembly and fluid instabilities in both bulk and nanoconfined environments.

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CHIRAL CRYSTALLIZATION OF AMORPHOUS TELLURIUM

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Tellurium (Te) is one of the very few inorganic materials having a chiral (in this case helical) crystal structure. However, the mechanism(s) by which chirality occurs on crystallization is unclear. In this talk, I will describe the results of computer simulations of the crystallization of glassy Te using a machine-learned (ML) interatomic potential to drive molecular-dynamics (MD) simulations of sufficiently large-scale (102, 000-atom) glassy Te models for long enough times (34 ns) to reveal the full chiral-crystallization process. It was discovered that transient cubic-like structural motifs, with lifetimes of only a few ns, act as intermediates in the creation of chiral crystal-like helical structures from the starting glassy phase, and they also mediate the transfer of chirality between right-hand and left-hand forms, both within chiral-crystal grains and between differently chiral grains at their grain boundaries.

The results of related simulations of the melting of crystalline Te will be described, in relation to the operational mechanism of the recently discovered use of Te as an electronic switch: the off-state is the semiconducting crystalline state; the on-state is the transient metallic liquid state. ML-MD simulations have shown that polycrystalline Te melts at a significantly lower temperature than the single-crystal form, thereby explaining why the first-fire Joule-heating drive voltage is significantly larger than the voltages need on successive switching cycles.

RELEVANCE BETWEEN MOLECULAR COOPERATIVITY AND NUCLEATION OF ORGANIC GLASSES

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Nucleation is the first step of nucleation. Although the nucleation process is generally explained by classical nucleation theory that considers balance of internal and interfacial energies, it is not sufficient to allow prediction of the nucleation process of glasses. Based on our series of investigations, molecular cooperativity is likely to play an important role for the nucleation. Ibuprofen glass has a glass transition temperature at −45°C. It does not crystallize during heating in differential scanning calorimeter; however, cold crystallization to form I was observed if it is annealed at nucleation temperature beforehand. The cold crystallization was the best enhanced when it was annealed at −15°C, which was regarded as the optimum nucleation temperature. On the other hand, characteristic length of cooperatively rearranging region was determined as a function of temperature using relaxation data obtained by broadband dielectric spectroscopy. It was compared with calculated critical size of nuclei to find that they coincident at ca. −15°C. This result indicated that nucleation was the most enhanced, when sizes of critical nuclei and cooperatively rearranging region coincide. The same procedure was applied to celecoxib glass to find that the nucleation temperature to form I was ca. 60°C. It agreed with the experimental observation that storage of celecoxib glass at 60°C cause crystallization to form I. These observations indicate importance of molecular cooperativity for inducing efficient nucleation of glasses.

Exploring in real time the thermal annealing of mixed amorphous optical coatings

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High-performance amorphous optical coatings, such as those forming the main mirrors in gravitational wave detectors, must be subject to a post-deposition thermal annealing. During this thermal process, the out-of-equilibrium structure of the amorphous coatings can relax and evolve towards a lower point in the energy landscape. The relaxation of optical coatings can be optimized by carefully tuning the annealing parameters, such as the maximum temperature, the annealing duration and the heating rate [1].
In this talk, I'm going to present the thermal annealing of $\mathrm{Ti:Ta_2O_5}$ and $\mathrm{Ti:GeO_2}$, the two most relevant oxide coatings currently considered for gravitational wave detector mirrors [2,3]. The effects of different annealing parameters on the thickness and refractive index of the two types of coatings are discussed. $\mathrm{Ti:Ta_2O_5}$ and $\mathrm{Ti:GeO_2}$ exhibited qualitatively different behavior upon annealing, pointing to different mechanisms at play once the annealing process has started. We ascribe the most remarkable variations observed in $\mathrm{Ti:GeO_2}$ – namely, a sizable thickness reduction when annealing temperature is raised up to 600°C - to the glass-forming properties of $\mathrm{GeO_2}$ [3]. Studying in real time the thermal annealing of amorphous optical coatings, as proposed in this talk, can unlock new insights in the thermal effects on out-of-equilibrium amorphous systems, and can be beneficial to enhance the performance of optical coatings for scientific and technological applications.

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Relaxation phenomena during chemical tempering of soda-lime silicate glass

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Chemical tempering based on ion exchange (potassium for sodium) is a crucial tool for improving the mechanical properties of glass artifacts by building up a compressive surface residual stress profile.

Herein, we investigated the chemical tempering of soda-lime silicate float glass between 380 and 490°C. The medium-range evolution was deeply investigated and correlated with the residual stresses and their relaxation.

It is shown that the glass undergoes 3 distinct stages during ion exchange, which depend on the ion exchange temperature: (i) the network behaves as a rigid framework where K-ions are incorporated, this causes a sensible drop in the free volume without an alteration of the bonding angles; (ii) increasing the temperature new sites becomes available for potassium, the potassium incorporation deforms the bonding angles of the silicate network and the free volume further decreases; under these conditions a maximum in the residual stresses is achieved; (iii) the residual stresses starts to relax from 460°C, this correlates with a relaxation of the bonding angles toward the equilibrium ones and an increase in the free volume. The strained and "out of equilibrium" network provides an additional excess in free energy, which sum up with the elastic one and is responsible for the relaxation phenomena.

These results contribute to a fundamental understanding of the stress relaxation phenomena during chemical tempering and correlate them with the glass structure.

THERMAL STABILITY OF ORGANIC SEMICONDUCTOR THIN FILM GLASSES BY LOCAL CHANGES IN SPONTANEOUS ORIENTATION POLARIZATION

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Vapor-deposited organic semiconductor glasses can exhibit pronounced molecular anisotropy and exceptional kinetic and thermodynamic stability if grown at proper conditions, compared to isotropic, poorly stable glasses formed by liquid quenching. Vapor-deposited glasses composed of organic molecules with permanent dipole moments generate a measurable surface potential due to this anisotropic molecular orientation. In this work, these properties are exploited to study local surface potential changes as a stable glass transforms into a supercooled liquid upon heating above the glass transition temperature (T_g). Local electrostatic force microscopy and Kelvin probe force microscopy are used to probe the dynamics of the phase transformation above T_g. The results demonstrate that polarization changes accompanying conversion to the isotropic liquid provide an effective proxy for tracking the transition and highlight their potential for assessing the thermal stability of organic devices under diverse thermal conditions.

Part III

Posters

LIGHT-INDUCED CAGING IN COLLOIDAL SUSPENSIONS

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We have developed an extension of mode-coupling theory for $(d+1)$-dimensional dense colloidal suspensions subjected to a one-dimensional periodic external potential [1]. As a case study, we investigate a system of hard disks and map out the nonequilibrium glass-transition diagram as a function of packing fraction and the period of the external field for various potential strengths [2]. Similar to systems under a washboard potential, the interplay between local packing effects and the commensurability of the external field period leads to distinct particle-caging geometries and gives rise to striking non-monotonic behavior in the glass-transition diagram as the field period is varied. This behavior enables both the melting of a glassy state and strong vitrification at moderate densities solely through tuning of the external field. These effects arise, respectively, from the incommensurability and commensurability between local packing and the imposed field periodicity. Notably, we identify regions in the nonequilibrium state diagram where moderate periodic modulation stabilizes the liquid state, whereas for other periods it stabilizes the glassy state. Overall, we show that these additional experimental control parameters provide a high degree of tunability over the liquid-glass transition by controlling the shape of local cages – an effect we refer to as *light-induced caging* [2].

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Effect of glass stability on the low frequency vibrations of vapor deposited glasses

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Ultra-stable glasses prepared from the physical vapor deposition of organic molecules present a very low density of two-level states, the kind of glass defects that determine their peculiar low temperature thermal properties [1,2]. Numerical simulations suggest that quasi-localized harmonic vibrational modes emerge in the soft regions associated with two-level states [3]. However, the connection between the low frequency vibrational modes and the local structural instabilities of glasses remains unexplained.

Here we exploit a recently developed spectrograph for nuclear resonant analysis of inelastic X-ray scattering [4] to probe the density of vibrational states of amorphous thin films of ultrastable and conventional glasses down to an exceptionally low frequency of 70 GHz [5]. We show that the glass stability does not affect the harmonic vibrational modes at the lowest frequencies, despite a reduction of almost an order of magnitude in the density of two-level states. At the same time, the vibrational modes at higher frequencies, around the boson peak maximum, are extremely sensitive to the glass stability. Although we cannot exclude the possible existence of quasi-localized modes in glasses, we show that their presence is not strictly necessary to describe the measured density of low frequency vibrations. The experimental developments here presented pave the way to the solution to the long-standing debate on the low frequency vibrations in glasses.

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IN-SITU XRD TRACKING OF STRUCTURAL CHANGES IN METALLIC GLASSES DURING THERMAL SCANS

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Understanding atomic-scale structural changes under varying thermodynamic conditions is essential for studying material properties and the mechanisms governing them, particularly in systems like glasses where thermal history plays a crucial role. To address this challenge, we developed a novel experimental setup that combines synchrotron X-ray diffraction (XRD) with fast scanning calorimetry (FSC) [1], providing high signal-to-background scattering measurements for in-situ characterization of nanoscale structural changes during and after rapid thermal scans. Experiments at the ESRF beamline ID15A on a Pd-based metallic glass ($Pd_{42.5}Cu_{30}Ni_{7.5}P_{20}$) show that the setup captures temperature-dependent structural changes during ultrafast FSC scans on the millisecond timescale and probes atomic-scale structural evolution is probed during aging treatments ranging from 0.5 T_g to above T_g. These results highlight the potential of the combined FSC–X-ray scattering approach to advance our understanding of the relationship between atomic structure and thermodynamics, thereby supporting future research in metallic glasses and other complex materials.

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CALORIMETRIC ANALYSIS OF DEPOSITED AMORPHOUS GeTe AND ITS RELEVANCE FOR PHASE-CHANGE MATERIALS APPLICATIONS

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Phase change materials (PCMs) are currently at the focus of an intense research effort as prominent candidates for revolutionary developments of universal memories and computation devices [1]. The transition between the two logic states (0 amorphous, 1 crystalline) is fast: few picosecond for erasing and tens of nanosecond for the writing, the latter process being the bottleneck to make PCMs compatible with the requirements for random access memories. Understanding the crystallization/amorphization process in detail is then a major line of research for these materials [1]. This work presents a study of deposited amorphous GeTe using new methods related to Fast Differential Scanning Calorimetry [2] to get information on the out-of-equilibrium state of the glass and on the crystal nucleation/growth kinetics. The effect of thermal treatments in a wide region below the glass transition temperature on enthalpy relaxation and the stability of the amorphous state has been carefully studied. These results could suggest a correlation between β-relaxation or fast processes active in the gassy state and crystallization kinetics [3].

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PREDICTING THE CRYSTAL GROWTH RATE AT THE SURFACE OF MOLECULAR GLASSES

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Organic glasses are capable of forming crystals on a free surface much more rapidly than within the bulk [1,2]: crystal growth can occur at a rate of few $\mathrm{nm\,s^{-1}}$ even $100\,\mathrm{K}$ below T_g. This behavior is commonly attributed to the elevated mobility of molecules at the surface [3], even though its origin is still debated. We here demonstrate that the slow Arrhenius process (SAP) [4,5], a microscopic mechanism that facilitates the reshaping of packings in amorphous systems, plays a significant role in enhancing surface crystal growth.

We propose a simple model able to predict how fast crystals grow on the surface of molecular glasses, based on a theoretical framework that characterizes the SAP through a series of collective small displacements [6]. Our model, requires as input, a simple thermodynamic characterization of the material. Anticipating a connection between orientational ordering, surface mobility, and the SAP, our work shows the potential of exploiting the latter to predict and tailor the properties and non equilibrium kinetics of glasses and crystals.

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COUPLING GROWTH STRATEGIES TO ORGANELLE PARTITIONING: NOISE EXPLAINS GENERATION-DEPENDENT BIASES IN CELL PROLIFERATION

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Partitioning noise describes the variability in the inheritance of molecules or organelles between daughter cells, arising from the stochastic processes involved in division [1]. While an homeostatic growth and division strategy is the rule by which a cell links growth and the division trigger so that cell sizes reach a stationary distribution in time. In this work we study how couplings between them may affect population-level observables in live proliferating cell populations [3]. We model single-cell size with exponential growth and a stochastic splitting-rate framework and implement division noise via a symmetric Gaussian-mixture. Gillespie simulations track generation-resolved dilution of an initial marker and are compared to the mean-field prediction [4]. For size-correlated components, broad partitioning generates systematic deviations in generation averages. This arises from coupling between birth-size asymmetry and division-time statistics: daughters inheriting larger fractions divide sooner, biasing late generations. Extending to two components with independent or correlated partitioning shows that correlation alone is insufficient; deviations appear only when asymmetric inheritance affects growth or division timing. To test these predictions and to interpret generation-resolved inheritance data we devised a flow-cytometry–based proliferation assay [4,5] for Jurkat leukemia and HCT116 colon adenocarcinoma cells.

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EXTRACTION OF REAL-SPACE CORRELATION FUNCTIONS FROM NEUTRON TOTAL SCATTERING EXPERIMENTS

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The processing of neutron total scattering data is a delicate task that involves a sequence of operations which must be carried out carefully, robustly, and – most importantly – reproducibly. The overall workflow can be naturally divided into three consecutive stages.

The first stage corresponds to data reduction, in which the raw detector counts are converted into diffraction patterns. This step is independent of the sample under study and involves only instrumental corrections, such as detector efficiency, normalization, background subtraction related to the instrument environment, and geometrical effects.

The second stage is the sample-dependent data correction, which relies on auxiliary measurements and detailed knowledge of the sample. This step allows the extraction of static structure factors that are free from experimental artifacts, including multiple scattering, absorption, inelasticity effects, and residual background contributions. At this level, the quality and consistency of the corrections directly impact the reliability of any subsequent real-space analysis.

The final stage consists of the analysis of the corrected structure factors and their transformation into real-space correlation functions. This typically involves Fourier transformation procedures, appropriate window functions to mitigate truncation effects due to the finite Q_{max}, and a careful assessment of systematic errors that may propagate into the pair distribution function.

In this contribution, we present a detailed description of this full workflow, with particular emphasis on the analysis stage for neutron total scattering experiments. The procedure is implemented using a dedicated Python module, ToScaNA (Total Scattering Neutron Analysis), specifically developed for this purpose. The method is based on an iterative approach that enforces the physical condition of the vanishing pair distribution function in the region of atomic repulsion at low-r. This constraint is used to self-consistently determine the contributions from multiple scattering, attenuation, and inelasticity effects. In addition, the approach provides a reliable and internally consistent estimate of the atomic number density of the system, which is a critical parameter for quantitative real-space analysis. The combination of physical constraints, iterative refinement, and reproducible numerical implementation makes this methodology particularly well suited for high-quality neutron total scattering studies across a broad range of disordered and partially ordered materials.

MONTE CARLO-BASED DESIGN OF AN INHIBITORY PEPTIDE TO IMPEDE PATHOGENIC DIMERIZATION IN A MISFOLDED ANTIBODY LIGHT CHAIN

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Immunoglobulin light chain (AL) amyloidosis is a condition correlating with the formation of insoluble aggregates in a varied range of tissues thus strongly impairing the patients' quality and expectancy of life. The hypervariable nature of some regions on the light chains make each case unique and highlight the need for personalized therapeutics to tackle such a patient-specific disease [1].

In this study, we focused on a pathogenic homodimer we previously obtained from a patient-derived light chain. By analyzing the dynamics and the interface of this dimer, we identified a 15-residue peptide with potential inhibitory activity [2]. The peptide was then refined using a Monte Carlo-based computational mutagenesis protocol that iteratively improved its sequence to maximize complementarity with the protein interface, taking into account shape, electrostatics, and hydropathy. The resulting optimized peptide is found to bind the monomer with a binding affinity comparable to that of the full pathogenic interface.

These results suggest that the designed peptide could be a suitable antagonist against pathogenic dimerization, and demonstrate that our computational workflow could provide a general framework for designing patient-specific inhibitory peptides against aggregation-prone proteins.

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COMPUTATIONAL APPROACHES TO DESCRIBE BIOMOLECULAR INTERACTIONS: EXPLORING THEIR IMPLICATIONS IN MOLECULAR DESIGN

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Molecular recognition relies on the fine-tuning of physicochemical properties at biomolecular interfaces. The increasing availability of experimental data on macromolecular complexes, at both the sequence and structure levels, has stimulated the development of computational approaches aimed at the compact and effective representation of molecular interfaces and the assessment of the stability and quality of their interactions. In this panorama, despite the huge progress observed in the field thanks to the introduction of artificial intelligence–based approaches, this problem still remains a major challenge in computational biology, particularly when it comes to evaluating the impact of single mutations on binding processes. Indeed, the development of reliable computational algorithms in this area would have significant implications, such as the rational design of molecular interfaces for ad hoc purposes.

I will describe the computational methods that I contributed to develop for the understanding of key interface properties, including interaction surface geometry, electrostatics, and hydrophobicity. These efficient formalisms enable the iterative evaluation of residue substitutions within a Monte Carlo simulation, generating multi-residue protein mutants with controlled binding compatibility. Finally, this method has been applied to molecular systems with high biomedical and biotechnological relevance, such as the design of peptides capable of interfere with pathological protein–protein interactions or the engineering of G protein–coupled receptors (GPCRs) to render them selectively responsive to user-defined molecules.

NMR STUDIES OF WATER AND ION DYNAMICS IN SYNTHETIC FLUORO-HECTORITE

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Investigating ion transport in solid material is a crucial part of developing robust devices for energy storage and sensors. Fluorohectorite, a clay mineral of the smectit group, serves as a model material for this investigation, specifically layered $Li_{0.5}[Mg_{2.5}Li_{0.5}]Si_4O_{10}F_2$ structure are of high interest in electrochemical devices due to their high ionic conductivity [2]. The charge transports results from interlayer lithium ions, which are dissolved in water. We uses ^{2}H and ^{7}Li NMR to study the temperature-dependent dynamics of the inter-layer water molecules and lithium ions. Diffusion coefficient measured using Static Field Gradient shows the 2-Dimensional nature of the transport. The effect of confinement strength on both local and diffusive dynamics were investigated by systematically varying the slit height [2]. We observe a reduction in diffusion coefficient for water compared to bulk under the influence of strong confinement. Water and Lithium ions exhibit distinct dynamics which is highly influenced by the clay surface. Combining information about diffusive and local dynamics allow us to study the applicability of the Stokes-Einstein relation and it makes NMR a versatile tool to understand the complex dynamics of the ions in the system.

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DESCRIPTION OF THE COMPLETE PHASE DIAGRAM OF GETE WITH A SINGLE MACHINE LEARNING POTENTIAL

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Phase-change materials (PCMs) are compounds that exhibit significant differences in electrical resistivity and optical properties between their crystalline and amorphous phases. These characteristics, combined with a fast crystallization rate, make them highly suitable for applications such as non-volatile memory devices, where short laser pulses are used to induce order–disorder phase transitions to write and erase information [1]. A well-known PCM is Germanium Telluride (GeTe). At ambient temperature, it adopts a crystalline rhombohedral phase [2]. When heated above 700 K, it transitions to a rock-salt crystal structure [3], and at temperatures above 1000 K, it becomes a liquid [4]. Here, in order to study the material, a machine learning potential is trained, validated and tested, employing the recently developed MACE architecture [5]. The dataset is constructed from snapshots of crystalline, liquid, and amorphous GeTe coordinates [6–7]. For each configuration, calculations of energies, forces, and stresses are performed within Density Functional Theory framework, employing the Quantum ESPRESSO suite [8–9–10]. Finally, a series of molecular dynamics simulations for GeTe is performed and analyzed. We show that the trained potential is accurate in all GeTe phases.

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QUANTITATIVE ASSESSMENT OF PHYSICAL AGING ON THE DYNAMICAL HETEROGENEITY OF AMORPHOUS ALLOYS: INSIGHT FROM STRESS RELAXATION

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Probing the dynamical and structural heterogeneity is a critical issue for understanding the mechanical and physical properties of amorphous alloys. Here, the stress relaxation of a $(La_{0.6}Ce_{0.4})_{65}Al_{10}Co_{25}$ amorphous alloy is investigated to probe the evolution of dynamical and structural heterogeneity due to aging. The characteristics of amorphous alloys are time-dependent during stress relaxation due to the inherent metastability; thus, the aging effect should be considered by modifying the classical Kohlrausch–Williams–Watts (KWW) function. Instead of constant parameters, the parameters of the KWW function are substituted by time dependent functions, as physical aging leads to an increase in the characteristic time and also produce a change in the stretched exponent . Our results find that the latter parameter decreases along aging, extending the stress relaxation curve towards long-times while, at the same time broadens the relaxation spectrum. The results demonstrated that the modified KWW function and the corresponding parameters conform to the conventional understanding of amorphous alloys.

A MODE-COUPLING THEORY OF THE GLASS TRANSITION FOR POLYDISPERSE SYSTEMS

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The glass transition in multicomponent colloidal suspensions has been investigated previously within the framework of the mode-coupling theory of the glass transition (MCT) [1,2]. Size-polydisperse systems are usually handled by approximating the particle-size distribution by a set of discretized species within MCT and are thus treated like multicomponent mixtures. This leads to a computational effort strongly scaling with the number of species. One could calculate the relevant quantities, but even by employing the symmetries of the system, this endeavour limits the maximum number of species by which the system can be represented. To tackle this limitation, we show the covariance of the Mori-Zwanzig equations and the mode-coupling functional in the species space and introduce a transformation matrix based on the particle sizes around the mean particle size [3]. Applying the transformation matrix allows for the direct computation of the intermediate scattering function (ISF) for the total density fluctuations. The higher-order total density fluctuations become increasingly less relevant, suggesting a cut-off approximation because the total ISF already contains the necessary information about the dynamics of the system. We compare the total ISF for a 10-component mixture against our results and show that already few modes in the new basis reproduce the relevant information quantitatively, drastically reducing computational complexity with reasonable accuracy.

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NMR STUDY ON THE DYNAMICS OF ICE IN BULK AND CONFINEMENT

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Nuclear magnetic resonance (NMR) and dielectric spectroscopy (DS) studies provided valuable insights into the defect-coupled and preparation-dependent molecular dynamics of hexagonal bulk ice [1-3]. While NMR revealed two dynamic processes, DS showed only one with a kink near 240 K. These processes were assigned to different types of defects in distinct temperature regimes.

To address this, we investigate molecular re-orientations using 2H NMR spin-lattice relaxation (SLR) and stimulated-echo (STE) measurements. In particular, we exploit the fact that STE experiments provide direct access to F2 rotational correlation functions, allowing us to probe the underlying dynamical mechanisms. The NMR results indicate contributions from Bjerrum defects and ionic defects, vacancies, or interstitials. To account for all observed effects, it is likely that we are observing a coupling of two defect types [4]. Moreover, we investigate dynamics in silica nanopores and gelatine-water mixtures. In these systems, ice coexists with a non-freezable layer of liquid water at the interfaces. Here, water crystallizes as stacking-disordered ice, consisting of interlaced cubic and hexagonal layers [5]. However, little is known about the dynamical properties of ice in nanoconfinements and mixtures. In particular, it is unclear which types of defects govern ice dynamics. We show that the rates and mechanisms of molecular reorientation depend on the confinement size and study the crossover to bulk behaviour.

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MODELING LIQUID–LIQUID PHASE DIAGRAMS OF THERMORESPONSIVE MATERIALS

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Desalination of seawater by forward osmosis is a technology potentially able to address the global water scarcity problem. The major challenge limiting its widespread practical application is the design of a draw solute that can be separated from water by an energetically efficient process. Here we investigate liquid–liquid phase separation of thermoresponsive ionic-liquid/water mixtures by molecular dynamics simulations. Two model systems are studied: tetrabutylphosphonium 2,4,6-trimethylbenzenesulfonate, [P_{4444}][TMBS], which exhibits a lower critical solution temperature, LCST, phase behavior, and protonated N,N,N-trimethylglycine, $[\text{Hbet}]^+$, bis(trifluoromethylsulfonyl)imide, $[\text{Tf}_2\text{N}]^-$, which displays an upper critical solution temperature, UCST, behavior. In both cases, down-scaling of the unit ionic-charges by a factor of 0.95 was necessary in order to reproduce qualitatively the temperature-composition phase diagrams. The magnitude of this factor, is much milder than those reported for ILs in neat phases, which can be explained by a diminished charge transfer, or induced dipoles, within the ions when the IL is in a mixture with water. With these models, the phase-diagrams are reproduced quantitatively. The chemical compositions of the spontaneously emerged phases are in excellent agreement with experimental findings. The critical temperature is overestimated by 5–10 K, and the viscosities are larger by a factor of 2–5, in comparison with experimental values.

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TEMPERATURE-DEPENDENT STRUCTURAL EVOLUTION IN A STRONG GLASSFORMER: THE CASE OF V-GeO_2

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The physical properties of a material are fundamentally determined by its atomic-scale structure. This relationship is especially important for disordered systems, which are pervasive in modern technology yet remain structurally less well understood than their crystalline counterparts.

In this poster, I will present my ongoing research on the temperature-dependent structural evolution of glassy GeO_2. The study combines isothermal neutron diffraction measurements collected at several temperatures between the glassy state (350 K) and the liquid state (1400 K) with structural modeling using Reverse Monte Carlo (RMC) methods. The initial configuration at 350 K is generated via Monte Carlo simulations employing the well-established Oeffner–Elliott potential and then refined against the neutron diffraction data. This refined structure is subsequently used as the starting configuration for the next temperature, enabling an iterative refinement procedure up to the liquid.

The resulting temperature-dependent structural models allow us to characterize both the short- and medium-range order at each stage, providing a detailed picture of how the structure of GeO_2 evolves from glass to liquid.

REVEALING HIERARCHICAL RELAXATION PATHWAYS DURING PHYSICAL AGING OF METALLIC GLASSES

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A fundamental challenge in understanding glass lies in unraveling the underlying mechanisms governing relaxation dynamics, especially as it relates to physical aging. For metallic glasses, the absence of long-range atomic order leads to pronounced non-equilibrium and non-linear aging dynamics. Gaining insight into the temporal or thermal evolution of configurational states during aging is not only crucial for accurately predicting the long-term stability of glassy states but also beneficial for guiding the design of amorphous materials. In this study, we investigate the relaxation dynamics of a $La_{60}Ni_{15}Al_{25}$ metallic glass, using both stress and enthalpy relaxation to elucidate the correlation between dynamical relaxation and equilibration kinetics. Enthalpy fictive temperature is applied as a key parameter to characterize configurational states, enabling a quantifiable measure of changes in relaxation time, activation energy and the dynamical heterogeneity as glassy system undergoes aging. A dual-step evolution of structural relaxation is observed, transitioning from an initial β relaxation-dominated phase to a regime more characteristic of α relaxation as the glassy system approaches equilibrium, reflecting the hierarchical nature of the energy landscape and the gradual stabilization of the amorphous structure. Our finding deepens the understanding of aging by integrating dynamic and thermodynamic perspectives, constructing a framework that links structural evolution to dynamic relaxation properties, which further offers key insights for the precision design of high-performance amorphous materials through strategic control of relaxation dynamics and structural states.

Index

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