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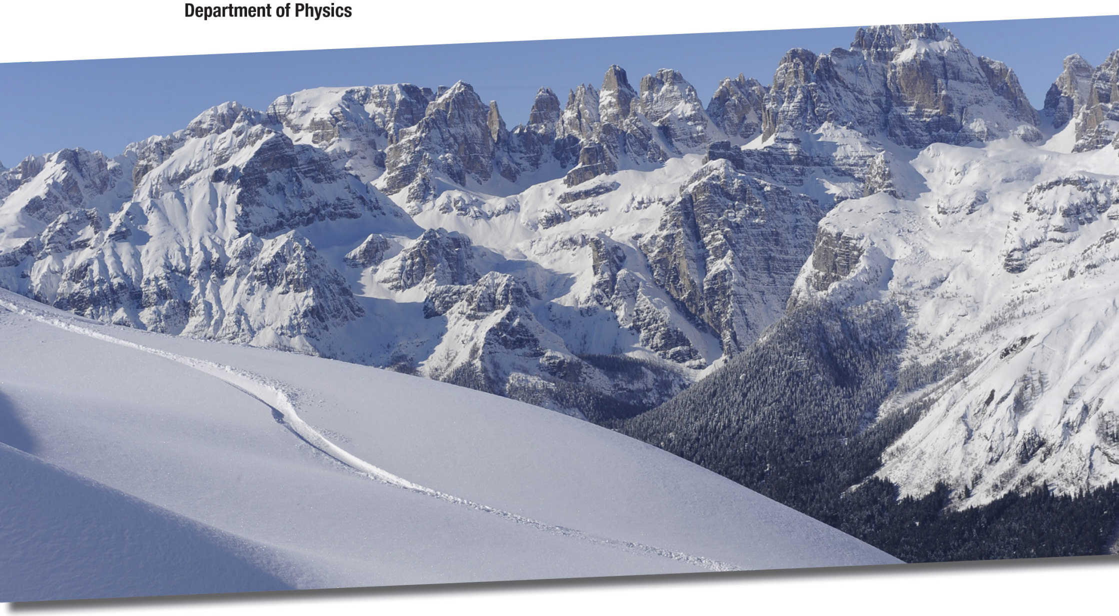

XIV International Workshop on Complex Systems

Fai della Paganella, Trento

March 22nd-25th, 2015

Book of abstracts

In memory of Paolo Verrocchio

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Part I

Programme

Sunday, 22 March

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18.20

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The enhancements of mobility at the surface and in thin films of polystyrene

Kia L. Ngai

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17.10

Solvent contribution to the stability of a physical gel characterised by quasi-elastic neutron scattering

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9.30

Dynamics of Molecular Associates in Methanol and Methanol/Water Mixtures

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9.50

Stability of linear asphaltene nanoaggregates in Cooee bitumen: a molecular dynamics study

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10.10

Gradient hydrogels with complex polymer structure obtained by one-step method

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A new surface model for two-component membranes

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16.50
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17.10
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18.05
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18.25
Times, Lengths and the Nature of the Glass Crossover
Tommaso Rizzo

18.45
Simple views on granular dynamics: jamming, bubbling, clogging, and meandering
Ko Okumura

19.05
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Thomas B. Schrøder

9.30
Explaining why simple liquids are quasi-universal
Andreas K. Bacher

9.50
Density scaling based equations of state
Andrzej Grzybowski

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11.00
Quantum Effects in the Glass Transition and Proton Conductivity
Alexei Sokolov

11.20
Voids, vibrations and relaxations in glasses
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11.40
How slow does a glass flow?
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12.00
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12.20
Glassy dynamics on a spherical substrate
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12.35
Mapping the structure of a glass throught its voids
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12.55

CONCLUSIVE REMARKS
Aldo Fontana & Giulio Monaco

Part II

Talks

DYNAMICS AND HETEROGENEITY IN RANDOM AND BLOCK COPOLYMERS OVER DIFFERENT LENGTH- AND TIME-SCALES

L. Andreozzi[1], M. Giordano[1], G. Galli[2], F. Zulli[1]

[1]Department of Physics "E. Fermi", University of Pisa, Pisa, Italy
[2]Department of Chemistry and Industrial Chemistry, University of Pisa, Pisa, Italy

In soft matter, liquid-crystalline polymers with photoresponsive azobenzene unit have attracted much attention as smart photonic materials because of their supramolecular self-assembled structures and their controllable properties in response to light. In particular, polymers containing azobenzene in side-chains are an ever expanding topic of both fundamental significance and practical potential, because the photoreaction of the chromophore is accompanied by a molecular reversible reorientation, generated from the molecular level over several spatial and temporal length scales.

Their peculiar functionalities make them eligible as high reliability rewritable media of light-induced nanowrited information or as all-polymer photonic microcavities. The performance crucially depends on parameters such as bit stability, homogeneity at molecular level, and working temperature [1,2].

In this paper, we report a study carried out by using different experimental techniques on a series of side-chain liquid-crystalline polymers, including homopolymers of an azobenzene methacrylate, and their random and block copolymers with varied amounts of methyl methacrylate counits. Their dynamics and matrix heterogeneity is discussed, highlighting how the different molecular architecture results in different dynamic responses and matrix heterogeneity.

[1] L. Andreozzi et al., Macromolecules **34**, 7325 (2001).
[2] L. Andreozzi et al., Macromolecules **46**, 5003 (2013).

STATISTICAL MECHANICS MODELS OF MULTIMODAL LASERS

F. Antenucci[1,2], A. Crisanti[1,3], M. Ibáñez Berganza[1,4], L. Leuzzi[1,2]

[1]Dipartimento di Fisica, Università di Roma "Sapienza", Rome, Italy
[2]IMIP-CNR, UOS Kerberos, Rome, Italy
[3]ISC-CNR, UOS Sapienza, Rome, Italy
[4]INFN, Gruppo Collegato di Parma, Parma, Italy

In this talk I will discuss the adoption of a statistical mechanics framework in optics. Two new models for multimode laser systems and their experimental implications are presented and critically analyzed. On the one hand, I will describe the solution of a mean field model for multimodal lasers in open and irregular cavities. The model includes the mode intensity dynamics and the presence of a linear coupling between the modes, due, e.g., to leakages from the open cavity. A replica symmetry breaking (RSB) transition is predicted at the random lasing threshold. For a high nonlinearity, a region with nonzero complexity anticipates the transition: in this case the light displays glassy behavior. Additionally, I will show that the RSB occurs also for the intensity fluctuation overlap, providing a feasible experimental test. On the other hand, I will present the first statistical mechanics models for passive mode locking beyond the mean field approximation. The model accounts for the presence of well-defined frequencies of the lasing modes inducing an inhomogeneous structure in the nonlinear interaction topology. By means of optimized Monte Carlo simulations, the system properties are analyzed varying interaction dilution, gain profile and number of modes. Novel properties of the resulting mode locked phase are presented: the topology inhomogeneity induces the appearance of phase waves with nontrivial slopes, resulting in a phase delay of the emitted electromagnetic pulse.

Explaining why simple liquids are quasi-universal

A.K. Bacher, T.B. Schrøder, J.C. Dyre

Glass and Time, Roskilde University, Roskilde, Denmark

It has been known for a long time that many simple liquids have surprisingly similar structure as quantified, for example, by the radial distribution function. A much more recent realization is that the dynamics are also very similar for a number of systems with quite different pair potentials. Systems with such non-trivial similarities are generally referred to as "quasi-universal". From the fact that the exponentially repulsive pair potential has strong virial potential-energy correlations in the low-temperature part of its thermodynamic phase diagram [2], we here show that a liquid is quasi-universal if its pair potential can be written approximately as a sum of exponential terms with numerically large prefactors. Based on evidence from the literature we moreover conjecture the converse, that is, that quasi-universality only applies for systems with this property. Our approach lays in continuation of recent results (see e.g. Refs. [2,3]).

[1] A.K. Bacher, T.B. Schrøder, and J.C.Dyre, Nat. Comm. **5**, 5424 (2014).
[2] A.K. Bacher and J.C. Dyre, Colloid Polym. Sci. **292**, 1971-1975 (2014).
[3] J.C. Dyre, Phys. Rev. E **88**, 042139 (2013).

Vibrational modes of glasses probed by inelastic X-ray scattering at the nanometer scale

G. Baldi

IMEM-CNR, Parma, Italy

Recent theoretical models for the vibrations in glasses assume that the complex elastic modulus depends on frequency but not on the wavevector, q. This assumption translates in a simple q dependence of the dynamic structure factor, which can be tested on the experiments. Following the suggestion of a recent paper [1], I present here a new analysis, performed in q-space, of inelastic X-ray scattering data on glasses. The outcome of the analysis is compared to the more common approach in the frequency domain and allows drawing some conclusions on the limits of validity of the mentioned theoretical assumption. I will then show that the spectrum of glass vibrations is similar to that of an assembly of polycrystalline aggregates of nanometer or sub-nanometer size, a length comparable to the extent of the medium range order of the glass [2]. The elastic modulus fluctuations occurring on this length scale are responsible for the strong damping of the sound waves [3] (Rayleigh scattering) and for the appearance of a plateau in the thermal conductivity at low temperatures.

[1] U. Buchenau, Phys. Rev. E **90**, 062319 (2014).
[2] G. Baldi et al., Phys. Rev. Lett. **110**, 185503 (2013).
[3] G. Baldi et al., Phys. Rev. Lett. **112**, 125502 (2014).

THE COMPLEX DYNAMICS OF A SIMPLE-MOLECULE LIQUID: METHANOL

S. Bellissima[1], F. Formisano[2], S. De Panfilis[3], E. Guarini[1], U. Bafile[4], M.A. González[5]

[1]Dipartimento di Fisica e Astronomia, Università di Firenze, Italy
[2]CNR-IOM, Grenoble, France
[3]Centre for Life Nano Science IIT, Roma, Italy
[4]CNR-ISC, Sesto Fiorentino, Italy
[5]Institut Laue Langevin, Grenoble, France

Methanol is a hydrogen-bonded liquid of enormous importance in pure and applied physics and chemistry, and is the object of innumerable studies. Yet, the fundamental aspects of its molecular dynamics are still known only to a very poor extent. The study of the collective dynamics is hindered by the weakness of the acoustic excitations, which has led to the wrong conclusion that sound modes propagate only in a surprisingly narrow range of small wave vector values. Combined molecular dynamics simulations and neutron Brillouin scattering measurements reveal, however, quite a different situation. Methanol is shown, for the first time, to feature the normal viscoelastic behaviour typical of a large variety of liquids, including the arrest of acoustic propagation near the peak of the static structure factor. Besides this, however, two more excitations are detected in the molecular centre-of-mass dynamics structure factor, at frequencies, respectively, one lower and one higher than the acoustic frequency, both with negligible dispersion. The rich translational dynamics revealed by this study classifies methanol as a fluid partly similar to, but possibly more complex than, water, where the presence of a second, low-energy, excitation is a long standing result although its interpretation has remained controversial for a long time. Moreover, the overall picture of the translational dynamics is enriched by interesting features visible in the single-molecule spectra.

NANOSCALE DYNAMICS BY EXTREME ULTRAVIOLET TRANSIENT GRATINGS

F. Bencivenga, R. Cucini, F. Capotondi, A. Battistoni, R. Mincigrucci, E. Giangrisostomi, A. Gessini, M. Manfredda, I.P. Nikolov, E. Pedersoli, E. Principi, C. Svetina, P. Parisse, F. Casolari, M.B. Danailov, M. Kiskinova and C. Masciovecchio

Elettra - Sincrotrone Trieste, Basovizza, Trieste, Italy

Four wave mixing (FWM) experiments are based on 3rd order coherent non-linear light-matter interactions and are used in the optical domain for a large array of applications. The possibility to use free electron lasers (FELs) to extend the FWM approach in the extreme ultraviolet (EUV) and x-ray range is attracting much attentions, also in light of the succesful demonstration of lower-order x-ray nonlinearities [1]. We report on the first observation of a FWM signal stimulated by EUV photon pulses [2], provided by the FERMI FEL facility in Trieste, as well as on the possibility to read its time evolution. This result paves the way for EUV/soft x-ray FWM, which, in the near future, would be used to study phonon-like modes in the unexplored wavevector (Q) range located above the range covered by visible-UV light scattering ($Q < 0.1$ nm^{-1}) [3]. Furthermore, EUV/soft x-ray photons can add atomic-site selectivity (through the exploitation of core resonances) to FWM methods and also allow probing excitations, such as valence band excitons, with energy comparable or exceeding that of optical photons [4]. These applications will be developed at FERMI in a dedicated experimental station, EIS-TIMER, which is expected to be available for users in 2016.

[1] N. Rohringer et al., Nature **481**, 488 (2012); M. Beye et al., Nature **501**, 191 (2013); T. E. Glover et al., Nature **488**, 603 (2013); S. Shwartz et al., Phys. Rev. Lett. **112**, 163901 (2014).

[2] F. Bencivenga et al., Nature (accepted).

[3] F. Bencivenga and C. Masciovecchio, MINA **606**, 785 (2009).

[4] S. Tanaka and S. Mukamel, Phys. Rev. Lett. **89**, 043001 (2002); F. Bencivenga et al., New J. Phys. **15**, 123023 (2013).

NEUTRON SCATTERING AND COMPUTER SIMULATION INVESTIGATIONS OF BIO-MEMBRANES IN WATER SOLUTIONS OF ROOM-TEMPERATURE IONIC LIQUIDS

A. Benedetto[1,2], P. Ballone[3]

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[2]School of Physics, University College Dublin, Ireland
[3]Center for Life Nano Science and Phys. Dep., Roma La Sapienza, Italy

The molecularly thin layer of water in direct contact with bio-molecules in a physiological environment plays a major role in determining their properties and functions. In this context, water is a shorthand notation for "water electrolyte solution", since almost without exception a variety of ions dissolved in water are needed to ensure the stability of bio-systems, greatly contributing to their complex behaviours.

In recent years, the development of compounds of the so-called room-temperature ionic liquid (RTIL) family has enormously expanded the number of ionic systems that could be used to modify the properties of the interfacial water, and thus to affect the behaviour of bio-systems.

Our study concerns the microscopic mechanisms underlying RTIL effects on biosystems through their hydration water, and relies on the combination of neutron scattering and molecular dynamics (MD) simulations.

We present the results for the interaction of imidazolium-based RTILs with phospholipid bilayers [1,2]. Neutron reflectometry and MD simulations confirm the tendency of cations to be absorbed into the lipid phase, enhancing the penetration of water into the bilayer. Neutron scattering and MD reveal apparent changes in the relaxation time of water in close contact of the lipid head upon addition of RTILs, that reflect phase changes in the structure and dynamics of the system.

[1] A. Benedetto et al., J. Phys. Chem. B **118**, 12192 (2014).
[2] A. Benedetto et al., J. Chem. Phys., submitted.

EVALUATION OF BRILLOUIN X-RAY DATA

U. Buchenau

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Making use of the classical second moment sum rule, it is possible to convert a series of constant-Q x-ray Brillouin scattering scans (Q momentum transfer) into a series of constant frequency scans over the measured Q range. The method is applied to literature results for the longitudinal phonon dispersion in several glass formers. The constant frequency scans are well fitted in terms of a Q-independent phonon damping depending exclusively on the frequency, in agreement with two recent theories of the boson peak. The method allows to link the x-ray Brillouin scattering to the diffuse Umklapp scattering from the boson peak vibrations at higher momentum transfer on an absolute intensity scale.

DYNAMICS AND STABILITY OF AMORPHOUS PHARMACEUTICALS UNDER DIFFERENT THERMODYNAMIC CONDITIONS

S. Capaccioli[1], D. Prevosto[2], M. Labardi[2], K.L. Ngai[3], W. Tu[3] and L.M. Wang[3]

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[2]CNR-IPCF, Pisa, Italy
[3]State Key Lab of Metastable Materials Science and Technology, Yanshan University, Qinhuangdao, Hebei, China

Glassy state improves the solubility and bioavailability of the active pharmaceutical ingredients (API), but the resulting excess free energy enhances their tendency to crystallize, limiting a safe long term storage. Recently, anomalous crystallization kinetics of molecular pharmaceuticals have been reported even near and below the glass transition temperature [1]. Despite extensive studies, a full understanding of the fast mode of crystal growth (FCG) in the glassy state is still missing [1,2]. Its presence was correlated to high fragility, strong translational/rotational decoupling and broad relaxation time distribution. The effect of density over thermal fluctuations in favoring FCG has been also proposed [2] but with controversial experimental validations [3]. The explanation for FCG could lie in mechanisms occurring at nanoscale [4] or connected to the local secondary relaxation. We present here a dielectric spectroscopy study of API dynamics under temperature and pressure variations, showing the relation of cooperative and local molecular mobility in bulk and at nanoscale with the stability against crystallization.

This study has been supported by MAECI-DGPSP within the Executive Program for Italy-China Scientific and Technological Cooperation (Significant Research Project PGR00137).

[1] Y. Sun et al., AAPS J. **14**, 380 (2012).
[2] T. Konishi et al., Phys. Rev. B **76**, 220201(R) (2007).
[3] K. Adrjanowicz et al., J. Chem. Phys. **136**, 234509 (2012).
[4] D. Musumeci et al., J. Phys. Chem. Lett. **5**, 1705 (2014).

A new setup for simultaneous Brillouin and Raman spectroscopy

S. Caponi[1], L. Comez[1], S. Corezzi[2], and D. Fioretto[2]

[1]CNR-IOM - Unità di Perugia, c/o Dipartimento di Fisica e Geologia, Perugia, Italy
[2]Dipartimento di Fisica e Geologia, Università di Perugia, Via A. Pascoli, I-06100 Perugia, Italy

The new set-up, recently built up at the GHOST laboratory, is a combination of a confocal microscope coupled with a tandem multipass Fabry-Perot interferometer and a TRIAX Jobin Ivon spectrometer. This home-made experimental apparatus allows us to simultaneously record micro-Raman and micro-Brillouin spectra achieving, in the same point of the analyzed sample, an in-depth structural and vibrational characterization. The huge frequency range accessible permits to simultaneously investigate the collective dynamics (longitudinal and trasversal acoustic modes at frequencies lower than 1 cm^{-1}), the Boson Peak (around 30-50 cm^{-1}) and the high frequency molecular vibrational modes (up to 4000 cm^{-1}) of a variety of samples. This setup presents a great versatility regarding the measurable samples, including opaque and heterogeneous materials. In this presentation, the instrument will be briefly described and its performances will be discussed reporting on different scientific cases.

UNDERSTANDING THE ATOMIC DYNAMICS AND THERMODYNAMICS OF GLASSES: STATUS AND OUTLOOK

A. Chumakov[1], G. Monaco[2]

[1]European Synchrotron Radiation Facility, Grenoble, France
[2]Dipartimento di Fisica, Università di Trento, Trento, Italy

The heat capacity of glasses at temperatures of about $\sim$ 10 K for a long time was considered to be anomalously higher than that of the corresponding crystals. The related excess of the low-energy vibrational states, the so-called 'boson' peak, was similarly considered to be an anomaly distinguishing glasses from crystals and related to their disordered state. Recent results [1] reveal that (i) the difference in the discussed properties occurs not because the glass is structurally disordered, but because it usually has lower density than that of the corresponding crystal, (ii) the heat capacity of glasses and crystals with same densities is quite similar, and (iii) the boson peak is the glassy counterpart of the van Hove singularity of the corresponding crystal. We analyze the generality of the new results and discuss the compatibility of the suggested interpretation of the boson peak with available experimental data. Analyzing the relation of the new results to various theoretical models, we discuss a possible experimental approach to explore further the nature of the low-frequency vibrational excitations in glasses [2].

[1] A.I. Chumakov, G. Monaco, A. Fontana, et al., Phys. Rev. Lett. **112**, 025502 (2014).

[2] A.I. Chumakov and G. Monaco, J. Non-Cryst. Solids **407**, 126 (2015).

ON THE COUPLING BETWEEN THE DYNAMICS OF BIOMOLECULES AND THEIR HYDRATION WATER IN THE TERAHERTZ REGION

V. Conti Nibali[1] and G. D'Angelo[2]

[1]Ruhr-University Bochum, Institute for Physical Chemistry II, Bochum, Germany
[2]Dipartimento di Fisica e Scienze della Terra, University of Messina, Messina, Italy

It is now widely recognized that hydration water in the proximity of biomolecules surfaces plays an essential role in the structure, stability, and dynamics of biomolecules. The significance of the spectroscopic information in the terahertz frequency range stems from the hydrogen bond network of water, which exhibits vibrational resonances exclusively between 1 to 6 THz, due to the numerous processes occurring in water on the picosecond time scale. On the other hand, biomolecular motions over this time scale are considered of primary importance for the fulfilment of dynamically driven biological functions. Therefore there is a growing interest in elucidating the dynamical coupling between biomolecules and their hydration water and in quantifying in which extent the dynamics of the solvent differ from those of liquid water as a consequence of this coupling. In this contribution we present a combined experimental and theoretical study of two model systems, i.e. a globular protein (MBP, maltose binding protein) and a model phospholipid membrane (DMPC, dimyristoyl-phosphatidylcholine) with the double aim of characterizing their terahertz vibrational dynamics and of elucidating the dynamical coupling with their hydration water.

AGING FLUCTUATION RELATION AND FLUCTUATION DISSIPATION THEOREM: A POSSIBLE RELATION

A. Crisanti

Dipartimento di Fisica, Università "Sapienza" di Roma, Roma, Italy

Non-equilibrium systems are characterized by a net energy transfer to the environment. Aging systems pertain to the category of weakly ergodic non-equilibrium systems exhibiting slow relaxational dynamics and strong history dependent effects. In contrast to stationary systems, aging systems are described by two timescales: the waiting time elapsed since the system was set in the non-equilibrium state and the measurement time. The hallmark of aging glassy systems is the violation of the fluctuation-dissipation theorem (FDT) and its two-slopes shape: 1 for short times, where the system is in (local) equilibrium and $x_{fdt} < 1$ for larger times. A characterization of the full spectrum of fluctuations appears key for a satisfactory understanding of the aging state. Over the past years several results about energy fluctuations in non-equilibrium states have been obtained under the heading of fluctuation theorem (FT). They take slightly different forms depending on the non-equilibrium context, but all share the same common feature: they relate probabilities of absorbing and releasing a given amount of energy under non-equilibrium conditions. Recently a fluctuation relation for the aging regime (AFR) of glassy systems has been introduced. Similar to the FDT, it defines a parameter $x_{af} < 1$ for the aging regime. Its connection with the parameter x_{fdt} obtained from Fluctuation Dissipation Theorem was based on numerical evidence. In this talk I will first review the definition of FT and the extension to the agin system deriving the AFR. Then I will show the emergence of the parameter x_{af} and its meaning. Finally I will discuss the relation between x_{af} and x_{fdt}.

VOIDS, VIBRATIONS AND RELAXATIONS IN GLASSES

C. Crupi[1], G. Carini[1], M. Gonzalez[2] and G. D'Angelo[1]

[1]Dipartimento di Fisica e Scienze della Terra, Università di Messina, Messina, Italy
[2]Institut Laue Langevin, Grenoble, France

A detailed investigation of the intermediate range structure on a series of alkaline and densified borate glasses has been carried out by performing room temperature neutron diffraction measurements. A cage model has been used to explain the compositional and pressure dependence of the first sharp diffraction peak in glasses. Our results are consistent with the hypothesis that the medium range order in glasses is related to the periodicity of the boundaries of cages in a random network of basic structural units. Furthermore we establish a correlation between the low frequency vibrational dynamics, the structural relaxation processes and the presence of voids on the nanometer length scale. The efficacy of this model has also been proved in several ring structured systems.

IS THE THZ DYNAMIC RESPONSE OF WATER REALLY ANOMALOUS?

A. Cunsolo

Brokehaven National Laboratory, Upton, New York, USA

Inelastic X-Ray and Neutron Scattering (IXS and INS, respectively) results on the mesoscopic dynamics of water will be reviewed illustrating a complex and rather peculiar phenomenology. In particular the focus will be on the onset of transverse wave propagation revealed by a low frequency peak in the spectrum of density fluctuations. It will be shown how two traditionally "rival" techniques, as IXS and INS, can be jointly used in a single experiment to gain deeper insight on the link between the THz viscoelasticity of water and its peculiar ability to support shear propagation over relatively large distances. Most important, the perspectives opened up by the construction of next generation IXS spectrometers will be illustrated in some detail.

PHYCHIP: LIVING DISORDERED SYSTEM FOR UNCONVENTIONAL COMPUTING

A. Dimonte, T. Berzina, V. Erokhin

Istituto dei Materiali per l'Elettronica e il Magnetismo, CNR, Parma, Italy

The slime mold Physarum polycephalum is a large cell visible by the unaided eye. Its growing behavior, with optimized patterns in configurations of attractants and repellents, can be interpreted as computation. Polyaniline (PANI) is a redox electro-chromic photopolymer highly studied, because of its interesting capability in changing conduction with a difference between the conducting and insulating forms of around 10 order of magnitude. Moreover, its electro-chromism rises in a color transition from transparent to yellow to green and blue, related to the addition/extraction of a proton. The same effect can be obtained with application of the adequate bias voltage as it is described in many works for the realization of organic memristors. Here we introduced a new system of creating networks with varied conductivity by interfacing the slime mold with PANI substrates. As a result, Physarum's growth changes the conductivity state of PANI layers in different ways, providing negative and positive patterning of the sample. Moreover, as an additional result, Physarum can act as an unconventional mask to transfer its designed networks on PANI substrates. What stands out is the creation of conductive channel designed by the mold but made by PANI.

QUANTITATIVE RELATIONS BETWEEN COOPERATIVE MOTION, EMERGENT ELASTICITY, AND FREE VOLUME IN MODEL GLASS-FORMING POLYMER MATERIALS

J.F. Douglas[1], F. Starr[2], B.A. Pazmino Betancourt[1]

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The study of glass-formation is largely framed by semi-empirical models that emphasize the importance of a progressively growing cooperative motion accompanying the drop in fluid configurational entropy, emergent elasticity, or the vanishing of accessible free volume available for molecular motion in cooled liquids. We investigate the extent to which these descriptions are related through computations on a model coarse-grained polymer melt with and without nanoparticle additives and for supported polymer films with smooth or rough surfaces, allowing a large variation of the fragility of glass formation. We find quantitative relations between emergent elasticity, the average local volume accessible for particle motion, and the growth of collective motion in cooled liquids. Surprisingly, we find that each of these models of glass-formation can equally well describe the relaxation data for all the systems that we simulate. In this way, we find some unity in our understanding of glass-forming materials from perspectives formerly considered as distinct.

DYNAMICS OF MOLECULAR ASSOCIATES IN METHANOL AND METHANOL/WATER MIXTURES

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The dynamics of molecular structures in methanol and methanol/water mixtures was investigated using quasielastic neutron scattering (QENS). These samples are notable cases of the many liquids[1] which, although homogeneous at the macroscopic level, present significant structuring at the nanoscopic level. By measuring the structure factor from samples differing only by their isotopic composition, structuring between methyl groups and hydroxyl groups (of both methanol and water) is put in evidence. Such structuring takes place over nano length scales which are however larger than the intermolecular distance. The dynamics of such molecular organization was studied by QENS taking advantage of the same isotopic substitution techniques. The data reveal that the molecular arrangement is transient but slower than the structural relaxation. In the pure methanol case the results can be

understood within the Transient Chain Model (TCM).[2] For methanol/water mixtures, the obtained dynamics over length scales of several nanometers is diffusive and significantly slower than the single particle diffusion of either methanol or water in the system. These results further validate the hypothesis of the existence of some structuring in the system[3] which is dynamic in character.

[1] Mesostructure and Dynamics in Liquids and Solutions, Faraday Discussion **167** (2013).

[2] C. Gainaru et al., Phys. Rev. Lett. **105**, 258303 (2010).

[3] S. Dixit et al., Nature **416**, 829 (2002).

If liquid-liquid transition can be observed in a water-glycerol mixture without ice formation?

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For the last decade the relaxation processes observed in wide frequency and temperature range in Water/Glycerol mixtures have been the subject of active discussion. Special attention has been paid recently to the low temperature region, where a first-order phase transition was detected at glycerol concentrations of about cg 20%mol. It was suggested that the phase transition is related to the Liquid-Liquid Transition (LLT) without a macroscopic phase separation. In this talk, we demonstrate that the observed transition is genuine ice formation. We show that water crystallization can occur only in a narrow water/glycerol concentration range, defined by the number of hydrogen bonds of glycerol molecule. Furthermore, in equilibrium water-rich mixtures the system can be in three different states: water molecules coupled to glycerol, bulk water pools or bulk ice particles (at low temperature), and interfacial water layers. The last are created between the water saturated glycerol matrix and volume ice. The origin of additional relaxation processes can be traced to dipolar interactions in the interfacial region. The interfaces of this region can be defined as *soft* or *hard*. Hard interfaces are largely inert to the influence of the water they are in contact with, while soft interfaces are more fluid, as there is a direct exchange with the surrounding water. We present the experimental measurements performed by BDS, DSC, XRD to support the proposed scenario. These results relate the observed phase transition to phase separation and water crystallization.

A molecular dynamics study of a 2D system of hard ellipses

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We have simulated the dynamics of a two dimensional system of hard ellipses by event-oriented molecular dynamics in NEV ensemble. Various quantities namely longitudinal and transverse velocity auto-correlation functions, translational and rotational diffusion mean squared displacements, pressure, intermediate self scattering function, radial distribution function and angular spatial correlation have been obtained and their dependence on packing fraction is characterized. Despite absence of prominent positional ordering, the orientational degree of freedom behaves nontrivially and exhibits interesting features. Slowing down is observed in the angular part of the motion near isotropic-nematic phase transition. It is shown that above a certain packing fraction the rotational mean squared displacement exhibits a three stage temporal regime including a plateau. Comparison to 2D system of hard needles is made and it is shown that from positional viewpoint, the ellipse system is more ordered.

DENSITY SCALING BASED EQUATIONS OF STATE

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The density scaling of molecular dynamics has been acknowledged as a valid unifying idea in the glass transition physics. The scaling behavior argued by the intermolecular potential based on the inverse power law has resulted in the power and general density scaling laws, which reduce dependences of dynamic quantities (e.g. structural relaxation times τ) on density ρ and temperature T to a single variable function $f(x)$ with $x = \rho^{\gamma}/T$ and $x = h(\rho)/T$, respectively, where the latter is not limited to $h(\rho) = \rho^{\gamma}/T$ with γ treated as a material constant. In search of a proper linkage between molecular dynamics and thermodynamics of supercooled liquids, we have recently derived equations of state (EOSs) [1,2], which comply with the power and general density scaling laws. We have validated the assumed theoretical grounds for the EOSs via molecular dynamics simulations and successfully applied the EOSs to describe experimental volumetric data of glass formers from different material groups, showing that the combined density scaling laws for and the total system entropy S underlie the EOSs. All the results allow us to claim that the density scaling based EOSs are good alternatives to the widely used phenomenological EOS formulated by Tait in 1888.

[1] A. Grzybowski et al., J. Phys. Chem. B **114**, 11544 (2010); Phys. Rev. E **83**, 041505 (2011); ibid. **86**, 031501 (2012).

[2] A. Grzybowski et al., J. Chem. Phys. **140**, 044502 (2014); M. Chorążewski et al., Phys. Chem. Chem. Phys. **16**, 19900 (2014).

NEW EXPERIMENTAL POSSIBILITIES ENABLED BY THE MATERIALS IMAGING & DYNAMICS (MID) INSTRUMENT AT THE EUROPEAN XFEL

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The Material Imaging & Dynamics (MID) Instrument at the European XFEL will enable X-ray scattering and imaging experiments on the nanoscale. Future users can benefit from hard X-rays in the energy range of 5-25 keV to investigate structural and dynamical properties in condensed matter with high spatial and temporal resolution.
The optical elements of the windowless beamline allow the transport of about 10^{16} photons/s in up to 10.000 pulses with an energy bandwidth of about 10^{-3} (SASE) or 10^{-4} (Self Seeding) and a duration of a few femtoseconds. Furthermore, two monochromators ($Si_{(111)}$ & $Si_{(220)}$) will be available. Based on different CRL focusing schemes, the focal spot can vary between hundreds of μm down to nanofocusing.
Scanning stages for solid samples, microfluidic setups as well as liquid & aerosol jets enable the investigation of different samples types and allow fast sample exchanges to comply with the high repetition rate of the XFEL. Additionally, the influences of constant and pulsed magnetic fields and/or optical excitation on samples can be investigated.
A special feature is the Split and Delay Line. Here, the FEL pulses are split and recombined through different sets of crystals. By changing the optical path length, one pulse part can be delayed compared to the other pulse part. This provides new experimental opportunities, e.g. X-ray pump/X-ray probe experiments and speckle visibility investigations on ultrashort time scales.

LOCAL ORDERING IN LIQUID METALS PROBED BY X-RAY ABSORPTION SPECTROSCOPY

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The nature of local point symmetry in simple monoatomic liquids has been a fundamental open question for almost 40 years of computational and experimental studies, following Frank's initial hypothesis about the presence of icosahedral short-range ordering (ISRO) in liquids. In recent decades, several computational and experimental studies were devoted to investigating locally preferred structures in simple atomic liquids and most of these works support the existence and importance of ISRO. We have performed an extensive investigation on liquid and undercooled liquid metals, combining state-of-the-art x-ray absorption spectroscopy (XAS) and computational techniques (Reverse Monte Carlo), for the purpose of evaluating the amount of ISRO, using reliable criteria for assessing the nature of local geometries in liquids (common-neighbor analysis, spherical invariants). We present original results of typical closed-packed metals (Cu, Ni) where the presence of ISRO is 10-14% embedded in a disordered network mainly composed of fragments of highly distorted icosahedra. New preliminary results of Cd and Zn are also presented, where ISRO is still present, but qualitative differences in the bond-angle distribution can be appreciated, showing a slight difference local ordering respect to the close-packed case.

NOVEL MAGNETIC EFFECTS IN NON-MAGNETIC GLASSES FROM THE STRUCTURE OF REAL GLASSES

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We propose a new cellular model for the atomic structure of real glasses, in which large better-ordered regions (containing micro-crystals in the case of the ceramic glasses) are packed in a distorted tetrahedral configuration. The particles in the interstices are responsible for the remnant dynamics of the otherwise dynamically arrested bulk. The dynamics can be quantum-mechanical at low temperatures (tunneling systems) or phonons thermally-activated closer to T_g. At low temperatures the model justifies local tunneling potentials containing up to four wells. The use of this extended tunneling model explains all reported magnetic effects in the cold glasses and predicts new ones in the acoustic attenuation coefficient and in the SQUID-magnetization, the latter effect being observable possibly also at higher temperatures. The implications of this approach for the nature of the glass transition will be discussed.

THE ORIGIN OF BOSON PEAK AND YANG-MILLS GAUGE FIELD THEORY FOR GLASSES AND SUPERCOOLED LIQUIDS

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Metallic amorhous-structures are described as resulting from competition between packing of the icosahedral clusters and the frustration by topological rules to attain global space filling. We have discussed the physical origin of the Boson peak, the viscosity of supercooled metallic liquid, melting, and the glass-transition in the gauge-invariant formula [1-7]. Especially the presence of the Boson peak is required naturally in the gauge-invariant condition. In this study, we shall discuss the detailed properties of the Boson peak,the relation between the breaking of duality symmetry of order-disorder parameters and glass-transition, comparison with other glassy materials as the high T_c cuprates [8], the diluted magnetic semiconductors [9], and perovsdkite manganites [10].

[1] I. Kanazawa, J. Non-Crst. Solids **150**, 2712 (1992).
[2] I. Kanazawa, Phys. Lett. A **176**, 1246 (1993).
[3] I. Kanazawa, Prog. Theor. Phys. Suppl. **126**, 397 (1997).
[4] I. Kanazawa, J. Non-Cryst. Solids **293-295**, 615 (2001).
[5] I. Kanazawa, J. Non-Cryst. Solids **312-314**, 608 (2002).
[6] I. Kanazawa, Radial. Phys. Chem. **58**, 457 (2000).
[7] H. Suzuki and I.Kanazawa, Intermetallics **18**, 1809 (2010).
[8] I. Kanazawa, Prog. THeor. Phys. Suppl. **157**, 107 (2005).
[9] I. Kanazawa, Physica E **29**, 647 (2005).
[10] T. Sasaki and I. Kanazawa, JPS Conf. Proc. **3**, 017001 (2014).

A new surface model for two-component membranes

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A new geometry-based surface model for two-component membranes is presented and studied by means of the Monte Carlo simulation technique on dynamically triangulated surfaces. In this model, variable σ is assumed to be the function of the metric degree of freedom on the triangles. The values of σ belongs to $\{1, -1\}$; this variable corresponds to the Euclidean metric and the induced metric. The Ising type interaction is assumed between the two nearest neighboring σ's on the triangles. It defines the aggregation energy and consequently the metric changes with the varying interaction coefficient λ. We find that the shape of the fluid surface becomes prolate/oblate for the large bending regions if λ is relatively big. The appearance of such anisotropic surfaces is due to the arising of domain structures in which the metric σ is uniform. These non-spherical forms are typical for the experimentally observed shapes in two-component membranes that are composed of two different lipids.

Stability of linear asphaltene nanoaggregates in Cooee bitumen: a molecular dynamics study

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Asphaltene and smaller aromatic molecules tend to form linear nanoaggregates in bitumen [1]. Over the years bitumen undergoes chemical aging and during this process, the size of the nanoaggregate increases. This increase is associated with an increase in viscosity and brittleness of the bitumen, eventually leading to road deterioration [2]. To prevent or reverse the effects of chemical aging, a first step is to gather more knowledge about the nanoaggregate structure and stability. In this talk, I will present the results of a detailed molecular dynamics (MD) study of a model bitumen: Cooee bitumen [3]. More specifically, the probability of having a nanoaggregate of a given size in the stationary regime will be quantified in MD and modelled. First, the simpler case where only asphaltene molecules are counted in a nanoaggregate will be modelled by a master equation approach and a related statistical mechanics model. The linear asphaltene nanoaggregates behave as a rigid linear chain. Second, the more complicated case where all aromatic molecules are counted in a nanoaggregate is discussed. The linear aggregates where all aromatic molecules are counted seem to behave as a flexible linear chain [4]. The case of branched nanoaggregates will be raised in the end.

[1] O.C. Mullins, Annu. Rev. Anal. Chem. **4**, 393 (2011).

[2] J.C. Petersen, Transportation Research Circular E-C140 (Transportation Research Board, 2009).

[3] J.S. Hansen, et al., J. Chem. Phys. **138**, 094508 (2013).

[4] C.A. Lemarchand et al., J. Chem. Phys. **141**, 144308 (2014).

MOLECULAR-DYNAMICS SIMULATIONS OF MECHANICAL REINFORCEMENT IN FILLED ELASTOMERS

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Rubber composites consist of a mixture of a pure elastomer and submicron size filler particles such as silica. At high volume fractions these particles form a reinforcing percolating network inside the polymer matrix, resulting in a much stiffer composite. Despite extensive work in the field, the origin of the reinforcement and its dependence on filler volume fraction has not yet been completely understood.

$Np_{zz}T$ molecular-dynamics simulations have been performed of a bead-rod polymer film confined between two crystalline substrates; the latter mimick the surfaces of the filler particles in a composite material. Different film thicknesses and different polymer-substrate interaction strengths have been simulated. The layer-resolved analysis of the polymer dynamics shows a tremendous slowing down of the mobility approaching the polymer-substrate interface, while the middle-layer exhibits bulk-like behavior. Upon decreasing the film thickness the mobility gradients become overlapping.

The rigidity of the films has been studied by simulating the elastic modulus from the linear regime of deformation normal to the film surface. A reinforcement was found compared to the bulk elasticity, increasing with an increase of the filler volume fraction and with increasing

strength of the adsorption. We connect this effect with the dynamic slowing down in the proximity of the fillers.
We also discuss the crosslinking effects on the thermomechanical properties of the simulated nanocomposite.

THE UNIVERSAL FRAGILE-TO-STRONG DYNAMICAL CROSSOVER AND THE ONSET OF THE SYSTEM VISCOELASTICITY

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The universality of the fragile-to-strong dynamical crossover (FSDC) in glass-forming liquids is discussed in the frame of the extended mode-coupling theory. The work stresses the importance for this phenomenon of the energy landscape concept for which the FSDC represents a sort of joint point between microscale and macroscale (e.g. how the understanding of mechanisms at the microscale can enable predictions of functional behavior at the macroscale). By using a molecular liquid (OTP) we give evidence that at the FSDC the Johari-Goldstein relaxation is observable and the system remains always ergodic. Whereas, by considering an attractive colloidal solution we observe the FSDC with the temperature and the density as control functions. This suggests that this dynamical transition influences the system viscoelasticity. Here we report the experimental evidence of this by means of a study of the colloidal system in a very large temperature-concentration interval. From the obtained findings and a comparison with scattering data on molecular systems (including also water) there is the suggestion that the Boson peak occurs at this special thermodynamical point, that on these bases may be considered more relevant than the qualitative definition of glass-transition.

TUNING INTERACTIONS OF IONIC LIQUIDS

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Ionic liquids (ILs) currently attract a large interest for a range of applications including energy technology, pharmaceuticals, and synthesis of new materials [1]. However, they are also of high interest from a more fundamental point of view. Being just made up of ions coulombic interactions naturally dominate, but due to the generally bulky nature of the constituent ions there is in most cases also a large contribution from van der Waals forces. There is now a general agreement that the presence of competing interactions is the cause for the presence of structural heterogeneities on the nm-length scale in ionic liquids. In this contribution we report on the evolution of structure and dynamics in both traditional ionic liquids and in so called solvated ionic liquids when the interactions are systematically tuned [2-3]. By doping the system with a Li-salt, with the same anion as in the IL but where the cation (Li) is small and very ionic, we can systematically increase the coulombic contribution to ion-ion interactions. Using a combination of Raman spectroscopy, small-angle x-ray scattering, dielectric spectroscopy and differential scanning calorimetry we follow how the local and mesoscopic structure as well as the dynamics is influenced by the altered interactions.

[1] A. Matic and B. Scrosati, MRS Bulletin **38**, 533 (2013).
[2] J. Pitawala, et al., Faraday Discuss. **154**, 71 (2011).
[2] J. Pitawala, et al., J. Non-Cryst. Sol. **407**, 318 (2015).

VIBRATIONAL EXCITATIONS AND ELASTIC HETEROGENEITIES IN DISORDERED SOLIDS

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Glasses feature inhomogeneous mechanical response at the nano-scale, i.e., some regions are sensibly softer than others. These *elastic heterogeneities* should interfere with the vibrational excitations supported by the material which, differently to the case of the perfect crystal, cannot be completely described in terms of phonons. In this work we have precisely addressed this issue by molecular dynamics simulations of a toy model, interpolating from the perfect crystal case, through increasingly defective phases, to fully developed glasses [1]. We have performed two independent series of calculations. On one side, we have determined the appropriate dynamical structure factors, and characterized the vibrational excitations in terms of frequency-dependent sound velocity and broadening [2], in analogy with experimental investigations. On the other, we have estimated the probability distributions of local elastic moduli and extracted the corresponding standard deviations [2,3], which are a direct measure of the extent of the elastic heterogeneity. By comparing the two sets of data, we have demonstrated a direct correlation between sound-waves features and the heterogeneous mechanical response at the nano-scale, without any adjustable parameter involved [3].

[1] L. Bocquet et al., J. Phys. Condens. Matter **4**, 2375 (1992).
[2] H. Mizuno, S. Mossa, and J.-L. Barrat, Proc. Natl. Acad. Sci. USA **111**, 11949 (2014).
[3] H. Mizuno, S. Mossa, and J.-L. Barrat, Europhys. Lett. **104**, 56001 (2013).

THE ENHANCEMENTS OF MOBILITY AT THE SURFACE AND IN THIN FILMS OF POLYSTYRENE

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Most of the studies of the dynamics at the surface and in thin films of polystyrene are focused on change of glass transition temperature from the bulk value. This purpose is served experimentally by techniques probing the segmental α-relaxation which is directly related to glass transition. Previously used techniques specifically for segmental α-relaxation include ellipsometry, Brillouin scattering, photon correlation spectroscopy and dielectric relaxation. Notwithstanding, creep compliance measurements by McKenna and co-workers [1] of high molecular weight polymer thin films probe not only the segmental α-relaxation but also the sub-Rouse and Rouse modes at higher compliance levels. Accompanying the reduction of the segmental relaxation time on decreasing film thickness is the dramatic decrease of the plateau compliance. The observed viscoelastic anomaly is caused by the sub-Rouse modes having their relaxation times also reduced in thin films, but to a much less extent than the segmental α-relaxation, and was explained theoretically in [2]. The creep compliance study of polymer thin films had brought out the difference in the responses of the various viscoelastic mechanisms at the surface and in thin films of polymers. More recently, viscous flow at the surface of low molecular weight polystyrene was measured by Chai et al. [3], and indirectly deduced by Yang et al. [4]. The viscosity at the surface was found to be reduced from the bulk value. It is important to recognize that for the low molecular weight polystyrene with $M_w = 3000$ g/mol used, viscous flow at the surface or in the bulk is carried out by the sub-Rouse modes, and not by the segmental α-relaxation. Therefore an explanation of the enhanced flow at the surface must come from the sub-Rouse modes. Since Chai et al. and Yang et al. made no connection of their surface flow data to the sub-Rouse modes, it is necessary to make this point in this paper. Also the lesses enhancement of mobility of the sub-Rouse modes than the segmental α-relaxation found from the creep compliance experiment explain also the reduction of viscosity at the surface is not as large as expected for the segmental α-relaxation. Earlier studies of dynamics of entangled polystyrene chains in high MW thin films are also considered.

[1] P.A. O'Connell, S.A. Hutcheson, and G.B. McKenna, J. Polym. Sci., Part B: Polym. Phys. **46**, 1952 (2008).

[2] K.L. Ngai, D. Prevosto and L. Grassia, J. Polymer Sci. B: Polym. Phys. **51**, 214 (2013).

[3] Chai et al., Science **343**, 994 (2014).

[4] Yang et al., Science **328**, 1676 (2010).

SIMPLE VIEWS ON GRANULAR DYNAMICS
– JAMMING, BUBBLING, CLOGGING, AND MEANDERING –

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In this talk, we will discuss three small-scale granular experiments, all prepared in quasi two dimension: (1) drag friction in a granular medium [1], (2) granular statics and dynamics in a certain hopper [2], and (3) meandering air flow in a granular medium [3]. For the drag friction, we highlight the divergence of the friction force towards the jamming point and a simple physical explanation for it. In the experiment, an obstacle is subject to friction in a two dimensional granular medium at packing fractions near the jamming point $\varphi = 0.841$. An average friction force acting on the obstacle is obtained as a function of the drag velocity at different packing fractions. The force and fluctuation both diverge towards the jamming point. The divergences are explained by a simple theory that demonstrates a clear data collapse. For the hopper problem, we discuss the statics of an unstable state and the dynamics of bubbles and its connection to clogging, again in simple physical frameworks. For the meandering problem, we discuss the mechanism of its destabilization and stabilization, together with a quasi-static nature. In all cases, we derive scaling laws for the phenomena on physical grounds, which all agree well with experiments.

[1] Y. Takehara and K. Okumura, Phys. Rev. Lett. **112**, 148001 (2014).
[2] Y. Yagisawa, and K. Okumura, in preparation.
[3] Y. Yoshimura, Y. Yagisawa, and K. Okumura, Phys. Rev. Lett. (under revision).

GRADIENT HYDROGELS WITH COMPLEX POLYMER STRUCTURE OBTAINED BY ONE-STEP METHOD

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Fast, one step method of manufacturing the polymer materials with linear gradient of properties will be shown. The hydrogels based on 2-(2-methoxyethoxy)ethyl methacrylate were prepared by electron-beam induced free radical polymerization with use of ethylene glycol dimethacrylate as additional crosslinking agent. Spectroscopic (Raman and NMR), imaging (SEM), goniometric and gravimetric techniques were used to find relationships between structure and physical properties of obtained materials at the macroscopic and molecular levels. The results indicated that the soft, highly swelled part of the gel, is significantly more hydrophilic and exhibit more homogenous structure in microscale in comparison with the hard part of the gel.

This project was supported by Polish National Science Center (grant no. 2013/09/B/ST4/03010) and Young Scientists' Fund at the Faculty of Chemistry, Lodz University of Technology.

[1] S. Kadlubowski, et al. Rad. Phys. Chem. **100**, 23 (2014).

COMBINING X-RAY CORRELATION SPECTROSCOPY WITH MICRO-TRACKING TO PORTRAY A 2D DYNAMICAL ARREST TRANSITION

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We report here an investigation of the slow fluctuation dynamics -on the scale of a few seconds- in a 2D model system made of silica nanoparticles (NP) interacting with phospholipid (DPPC) monolayers. We combine techniques operating in the direct space (micro-tracking) and in the reciprocal space (GI-XPCS) to characterize the dynamical regimes of this system. NP's presence induces significant modifications in the pristine phospholipid monolayers: in the pressure-area Langmuir isotherm, the coexistence plateau between liquid compressed (LC) and liquid expanded phases disappears and the morphology is characterized by round features, which are the phantoms of LC domains. At high surface pressure, these circular features form a closely packed, gel-like arrested state. Correspondingly, upon increasing surface compression, we observe a smooth and controlled evolution from Brownian diffusion to heterogeneous arrested dynamics, featuring intermittent ballistic-like rearrangements. This is indicated by direct tracking of the dynamics and it is confirmed by a detailed analysis of the GI-XPCS results, e.g. the shape of the correlation function and the relaxation time's dependence from the scattering vector.

IN LOOKING FOR A UNIVERSAL BEHAVIOR PATTERN FOR THE LIQUID FRAGILITY IN VARIOUS TYPES OF MATERIALS AND DIFFERENT THERMODYNAMIC CONDITIONS.

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The molecular studies of glass-forming liquids at elevated pressure become now a standard practice in many laboratories all over the word [1]. The addition of pressure as an external thermodynamic variable open a new perspective in understanding the fragility concept. The objective of this presentation is to show that the relaxation dynamics of van der Waals liquids, polymers and ionic liquids exhibit a uniform pattern of behavior when it is analyzed in terms of fragility concept. Consequently general rules defining the behavior of isobaric, isothermal and isochoric fragilities are formulated for these three groups of materials [2]. Our findings are consistent with the density scaling concept. Finally, it is experimentally proved that both isothermal and isobaric fragilities are new isomorphic quantities in the power low density scaling regime.

[1] G. Floudas, M. Paluch, A. Grzybowski, and K. Ngai, *Molecular Dynamics of Glass-Forming Systems: Effects of Pressure*, Springer-Verlag Berlin Heidelberg 2011.
[2] M. Paluch et al., J. Chem. Phys. **141**, 134507 (2014)

Hopping and dynamic phase coexistence in glass-formers

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Glass-forming materials are characterized by an intermittent motion at the microscopic scale, since particles diffuse through rare jumps out of the cages formed by their neighbours. A puzzling issue concerns the relationship between this cage-jump motion and the heterogeneous dynamics observed at larger length and time scales.

To this aim, we investigate cage-jump motion in numerical simulations of different glass forming systems and experiments of hard-sphere colloids, analyzing the particle trajectories via a novel parameter-free algorithm. In this talk, I'll show that single particle jumps are short lasting irreversible events leading to relaxation of the system and therefore they enable a description of glassy dynamics as a Continuous Time Random Walk. This framework allows a short time prediction of the diffusion constant and to relate the distribution of particle diffusivities to the distribution of the number of jumps per particle. In the deeply supercooled regime, the distribution of the single particle diffusion coefficients acquires a transient bimodal shape which provides the first direct observation of the dynamic coexistence of two phases with different diffusion coefficients. We relate the features of this distribution to the heterogeneity of the dynamics and to the breakdown of the Stokes-Einstein relation.

[1] R. Pastore et al., Soft Matter **10**, 5724 (2014).
[2] R. Pastore et al., Soft Matter **11**, 622 (2015).
[3] R. Pastore et al., arXiv:1412.5304 (2014).

SOLVENT CONTRIBUTION TO THE STABILITY OF A PHYSICAL GEL CHARACTERISED BY QUASI-ELASTIC NEUTRON SCATTERING

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Physicals gels formed by low molecular weight organic gelators (LMMOG) are composed of a rigid network formed by the gelators, in which is trapped a large quantity of solvent. The subtle interplay of the different forces exerted between the solvent and gelators enable the gels to reversibly assemble in a restricted temperature range in a complex structure that depends on the solvent. The dynamics methyl-4,6-O-benzylidene-α-D-mannopyranoside (α-manno) [1] in water and toluene are probed by neutron scattering [2]. The α-manno is an amphiphilic gelator that adopts different organisation inboth solvents. We were able to determine, on a timescale from a few ps to 1 ns, the number of solvent molecules that are immobilised by the rigid network formed by the gelators. We found that only few toluene molecules per gelator participate to the network which is formed by hydrogen bonding between the gelators' sugar moieties. In water, however, the interactions leading to the gel formations are weaker, involving dipolar, hydrophobic or $\pi - \pi$ interactions and H-bonds are formed between the gelators and the surrounding water. Therefore, around 10 to 14 water molecules per gelator are immobilised by the presence of the network. This study shows that neutron scattering can give valuable information about the behaviour of solvent confined in a molecular gel.

[1] O. Gronwald et S. Shinkai, Chem. Eur. J **7**, 4329-4334 (2001).
[2] I. Morfin, et al., Langmuir (2015), DOI: 10.1021/la5045656.

HYPERBRANCHED POLYMERS UNDER CONFINEMENT: AN INSIGHT BY CONVENTIONAL AND SPATIALLY RESOLVED DIELECTRIC INVESTIGATION

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Dendritic polymers constitute a relatively new class of materials that have attracted the scientific interest since their unique features like high density, low viscosity, and multiplicity of functional end-groups make them favorite candidates for numerous applications. Hyperbranched polymers, HBP, share the same features of dendritic macromolecules having the

additional advantage of a cost-effective synthesis, as compared to dendrimers. They can be used in many industrial applications, in particular in pharmaceutical industry and medicine for encapsulation as well as targeted delivery of drugs. Encapsulation and drug delivery are related to both the structural and dynamic properties of the polymer. In particular, polymer dynamics can be investigated by dielectric spectroscopy on the time scale from nanoseconds to months. Furthermore, a subject of great interest during the recent years is the study of dynamic behavior of polymer close to interfaces and/or in very thin films.
In this work, relaxation dynamics of the HBP Boltorn H20 has been investigated both in pure matrix and nanocomposites clays of montmorillonite (MMT) type. Conventional dielectric spectroscopy techniques have been used to investigate both the bulk matrix and nanocomposite materials. Dielectric spectroscopy at the local scale, performed by scanning probe methods, has been used to investigate the dynamics of nanocomposites. Polymer relaxation has been investigated in the same material close to the interface with MMT as well as far from it. The comparison of the results from the two techniques allowed to understand in more details the relaxation dynamics observed in the bulk material, as well as the complex interfacial interaction occurring within it.

Do Two-Level-Systems and boson peak persist or disappear in highly-stable glasses?

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We have studied how very deep kinetic and thermodynamic stabilization in glasses can affect their universal properties at low temperatures. In particular, we have investigated two different kinds of material which allow us to access highly-stable glassy states, as well as their corresponding conventional glasses: (i) ancient amber, which is a glass which has experienced an extremely long hyperaging process; and (ii) ultrastable thin-film glasses of indomethacin, prepared by physical vapor deposition at temperatures around 85% of its glass-transition temperature. Specifically, we have studied 110-million-year-old amber samples from El Soplao (Spain). Specific heat C_p measurements of pristine and rejuvenated samples were conducted in the temperature range 0.07 K$< T < 30$ K, as well as around its glass-transition temperature $T_g = 150$°C. A modest increase of the boson-peak height (in C_p/T^3) with increasing rejuvenation was observed. The amount of two-level systems (TLS) was however found to be exactly the same for the pristine hyperaged amber as for the subsequently rejuvenated samples. On the other hand, we have observed an unexpected suppression of the universal TLS in the ultrastable glass of indomethacin, whereas conventionally prepared thin films of the same material exhibit the usual linear term in C_p below 1 K, usually ascribed to TLS in glasses.

Dynamical anomalies in hot dense water

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Recent incoherent neutron scattering measurements [1] highlighted two unexpected anomalies in the diffusive behaviour of water in the high-pressure (> 1 GPa) and high-temperature (> 350 K) regime: the molecular diffusion coefficient deviates from the prediction of the Stokes-Einstein (SE) relation and the rotational diffusion is almost insensitive to pressure variation. Both anomalies were tentatively related to the peculiar behavior of the H-bond network relaxation under high density conditions[1] in contrast with a structural transition interpretation based on IXS and Raman data [2,3]. We thus performed new IXS and Raman measurements in the same $p - T$ regime, which confirmed that the SE break down can be attributed to the free volume reduction and the consequent onset of hopping phenomena while the invariance of the reorientational time is a consequence of the unchanged number and strength of the H-bonds per water molecule in the high density regime [4,5].

[1] L.E. Bove et al., Phys. Rev. Lett. **111**, 185901 (2013).
[2] M. Krish et al., Phys. Rev. Lett. **89**, 125502 (2002).
[3] T. Kawamoto et al., J. Chem. Phys. **120**, 5867 (2004).
[4] U. Ranieri et al., in preparation (2015).
[5] S. Fanetti et al., J. Phys. Chem. Lett. **5**, 235-240 (2014)

Slow dynamics of dilute polymers on energetically heterogeneous surfaces: a non-linear tale

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The behaviour of polymers on solid surfaces is important from both fundamental and technological perspectives. We will discuss the results of molecular dynamics simulations of a dilute layer of bead-and-spring polymers on randomly functionalized substrates, characterized by different fractions of weakly and strongly attractive sites [1]. Due to energetic disorder, we find a non-trivial dependence of several dynamical properties on surface composition. The activation energy for polymer diffusion is maximum when the fraction of strongly absorbing sites is $f = 0.75$ [2] The dynamics slow-down on cooling resembles that of a strong glass-forming liquid [3]. Like the activation energy, the estimated glass transition temperature is also maximum for $f = 0.75$. Our findings have a potential impact on polymer friction, adhesion and nancomposites. Future work will mainly concern the behaviour at higher polymer densities, where cooperative effects are expected to become increasingly relevant.

[1] G. Raos and T. J. Sluckin, Macromol. Theory Simul. **22**, 225-237 (2013).

[2] G. Raos and J. Idé, ACS Macro Lett. 3, 721-726 (2014).

[3] R. Pastore and G. Raos, submitted.

TIMES, LENGTHS AND THE NATURE OF THE GLASS CROSSOVER

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Stochastic Beta Relaxation (SBR) is a rather intuitive dynamical model of the glass crossover that has been derived by a dynamical-field theoretic treatment of Mode-Coupling-theory (MCT) near its dynamical singularity. We have performed a detailed numerical study of the solutions of SBR obtaining a comprehensive characterization of the glass crossover.
Both above and below the dynamical arrest temperature the density-density correlator decays from the plateau value as $-B(x)t^b$, where b is the same of MCT while the space-dependent prefactor $B(x)$ is due to the local random fluctuations of the temperature that are the main feature of SBR. From the $B(x)$ profile one can extract many important quantities, the α-relaxation time, the diffusion coefficient and the correlation length. We see that, approaching the critical temperature things changes with respect to ideal MCT: (i) dynamical arrest is avoided but (ii) the relaxation time starts to grow much faster, from power-law to exponential.
Dynamical fluctuations are naturally associated to fluctuations of the B-profile.The structure of dynamical fluctuations also displays an important qualitative change upon crossing T_{MCT}. Above T_{MCT} there is a power-law increase of dynamical fluctuations and of the dynamical correlation length. Below T_{MCT} strong *Dynamical Heterogeneities* appear as rare faster regions that dominate the global relaxation. Note that dynamics slows down because these regions are rare in space, but not because they are larger. Indeed the dynamical correlation length *decreases* slightly below T_{MCT} and decorrelates from the relaxation time. Overall the structure of dynamical fluctuations changes from being scale-invariant above T_{MCT} to being activated-like below T_{MCT}. As a consequence observables that scaled similarly above T_{MCT} decouple below T_{MCT} and this is reflected e.g. in deviations from the Stokes-Einstein relationship. We note that SBR cannot sustain too large fluctuations and could

fail well below T_{MCT}. There it could be replaced by activated dynamics characterized by elementary events with intrinsic time and length scales of an unusual large (but not necessarily increasing) size (mesoscopic vs. microscopic).

[1] T. Rizzo, Europhys. Lett. **106**, 56003 (2014).
[2] T. Rizzo and T. Voigtmann, (2015) arXiv:1403.2764 and to appear.

HYDROPHOBIC/HYDROPHILIC EFFECTS IN THE HYDRATION DYNAMICS OF POLYSACCHARIDE HYDROGELS BY UV RAMAN SCATTERING

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The hydration dynamics in a paradigmatic model of polysaccharide hydrogel is here explored by exploiting the combined use of UV Raman scattering and IR measurements. The case example of cyclodextrin nanosponges (CDNS)/hydrogel is chosen since the simultaneous presence in the structure of the polymer matrix of both hydrophilic and hydrophobic sites mimics the complexity of polysaccharide hydrogels. In this way, the contributions provided by the balance between the hydrophilicity/hydrophobicity to lead to the formation of the gel phase are separately accounted and evaluated. At the same time, we probe the molecular connectivity of water molecules confined in the pores of hydrogel trough the analysis of the vibrational spectra of CDNS hydrated with water and deuterated water. As main results, we found that the hydrophobic CH groups inserted on the aromatic ring of CDNS experience a more pronounced dynamic perturbation with respect to the carbonyl groups due to the collision between the solvent and vibrating atoms of the polymer. In a parallel way, we find a strong experimental evidence of a liquid-like behaviour of water molecules confined in the nano-cavities of hydrogel. The overall results provide a detailed molecular picture of the gelation phenomena occurring when a chemically cross-linked polymer contacts with water or biological fluids.

[1] B. Rossi et al., Phys. Chem. Chem. Phys. **17**, 963–971 (2015).
[2] B. Rossi et al., J. Chem. Phys. **142**, 014901 (2015).

DYNAMIC SUSCEPTIBILITY OF MOLECULAR AND IONIC LIQUIDS AS WELL AS POLYMERS

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Depolarized light scattering spectra of molecular and ionic liquids are studied by applying double monochromator and tandem-Fabry-Pérot interferometry (DM/TFPI). Combining these techniques with state-of-the-art photon correlation spectroscopy (PCS), broad band suscep-tibility spectra become accessible which can compete with those of dielectric spectroscopy (DS). Temperatures from T_g up to the boiling point T_b are covered (for molecular liquids) and the crossover from glassy to simple liquid dynamics is monitored. It is characterized by a merging of primary relaxation (α-process) and vibrational excitations and appearance of an Arrhenius law for $\tau_\alpha(T)$. The DM/TFPI spectra are interpolated by the F_{12} model of mode coupling theory.
In addition to $\tau_\alpha(T)$ the high-temperature spectra are characterized by stretching parameter β_{CD}, strength of fast dynamics $1-f$, and short-time scale expressed by an apparent moment of inertia I^*. For a given liquid the spectral parameters are virtually temperature independent up to T_b, i.e., frequency-temperature superposition applies. No correlation among β_{CD} and fragility is revealed. Attention is given to the evolution of the excess wing (or intermediate power-law) which appears upon cooling and is probed by DM/TFPI as well as PCS and NMR. The probe-dependent stretching of the α-process may be explained by a probe-dependent amplitude of the excess wing. The additionally observed slow β-process manifests itself rather universally in NMR and DS, but not at all in PCS experiments. Regarding molecular vs. ionic liquids, no relevant difference in the evolution of their spectra is observed.
Concerning the temperature dependence of τ_α, by decomposing the activation energy $E(T)$ in a constant high-temperature value E and a 'cooperative part' $E_{coop}(T)$, the latter depending exponentially on temperature, a 'generalized Angell plot' $E_{coop}(T)/E$ vs. T/E is introduced. Thus instead of the conventionally defined T_g it is suggested that E controls the energy scale of the glass transition phenomenon. The difference between polymers and molecular liquids lies in the fact that the ratio $E/E_{coop}(T_g)$ is systematically higher than those of molecular liquids, i.e., the temperature dependence of transport coefficients of polymers shows an Arrhenius behavior extending over a larger temperature range. Moreover, the molar mass dependence $E_\infty(M)$ saturates for polymers while it continuously grows for molecular liquids along $E_\infty(M) \propto M$ with $\alpha \cong 0.5$.

Theory of Heterogeneous Viscoelasticity

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We present a new theory of viscoelasticity of a glass-forming viscous liquid near and below the glass transition. In our model we assume that each point in the material has a specifc viscosity, which varies randomly in space according to a fluctuating activation free energy. We include a Maxwellian elastic term and assume that the corresponding shear modulus fluctuates as well with a similar distribution as that of the activation barriers. The model can be mapped to an effective heterogeneous elasticity theory, which is solved in

coherent-potential approximation (CPA). The theory predicts an Arrhenius-type temperature dependence of the viscosity in the vanishing-frequency limit, independent of the distribution of the activation energies. It is shown that this activation energy is generally different from that of a diffusing particle with the same barrier-height distribution.
At finite, but low frequencies the theory describes low-temperature alpha relaxation together with the beta wing. Good agreement with data on metallic glasses is obtained. At high frequencies the theory reduces to heterogeneous elasticity theory, which explains the occurrance of the boson peak and related vibrational anomalies.

Isomorph Theory v2.0

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The isomorph theory predicts for *Roskilde-simple liquids* the existence of *isomorphs*. These are curves in the phase diagram along which structure, dynamics, and some thermodynamic properties are invariant, implying that the phase diagram is effectively one-dimensional with respect to many reduced-unit properties. Here, the isomorph theory is reformulated [1] by defining Roskilde-simple systems by the property that the order of the potential energies of configurations at one density is maintained when these are scaled uniformly to a different density. Isomorphs remain curves in the thermodynamic phase diagram along which structure, dynamics, and excess entropy are invariant. In contrast to the original formulation of the isomorph theory, however, the density-scaling exponent is not exclusively a function of density and the isochoric heat capacity is not an exact isomorph invariant. A prediction is given for the latter quantity's variation along the isomorphs. Molecular dynamics simulations of the Lennard-Jones and Lennard-Jones Gaussian systems validate the new approach.

[1] T.B. Schrøder and J.C. Dyre, J. Chem. Phys. **141**, 204502 (2014).

How slow does a glass flow?

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Does the glass cease to flow at some finite temperature? Answering this question -of pivotal importance for glass transition theories- would require ridiculously long observation times. We recently demonstrated a way to circumvent this infeasibility, by relating the directly inaccessible ultra-viscous flow of a liquid to the elastic properties of the corresponding glass, which we measure as function of its age [1]. The older is the glass the lower is the temperature at which viscosity can be determined. Taking advantage of physical vapor deposition, we rapidly obtain a wide spectrum of ages rivaling those of millenary ambers, enabling viscosity determinations at values as large as those pertaining to the asthenosphere. Our result rules out the finite temperature divergence of the molecular diffusion timescale in a glass.

[1] E.A.A. Pogna, C. Rodriguez-Tinoco, G. Cerullo, C. Ferrante, J. Rodriguez-Viejo and T. Scopigno. Proc. Natl. Acad. Sci. USA **112**, 2331-2336 (2015)

TERAHERTZ DYNAMICS OF AMORPHOUS (BIO)PHARMACEUTICAL MIXTURES

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Previous terahertz studies of amorphous systems focused on understanding of the fundamental origin of terahertz losses and its behavior with temperature [1]. It has been shown that the losses in the terahertz region originate from both vibrational and relaxational response of the molecules. With this interplay in mind terahertz spectroscopy has proven itself as a very useful technique in describing the molecular mobility in amorphous systems. This has led to a discovery of a crystallization enhancement in amorphous naproxen around $0.67T_g$, most likely originating from the fast secondary relaxation [2]. Such results are very important for the formulation strategies of poorly soluble systems where amorphous state could be used to aid their solubility, such as pharmaceutical products. The present study provides more robust results on pharmaceutical and biopharmaceutical formulations. We have performed studies on amorphous polymer/drug mixtures of PVP-VA and paracetamol. By analyzing the terahertz response of different mixture concentrations we extracted information on the overall system stability, allowing for the optimal formulation strategy. Motivated by the work of Cicerone [3] we also performed a similar study on sugar glassy matrices of trehalose, where addition of small glycerol molecules may enhance the overall stability of the glassy matrix and lead to a better preservation of lyophilized proteins.

[1] J. Sibik, S. R. Elliott, J. A. Zeitler, J. Phys. Chem. Lett. **5**, 1968-1972 (2014).
[2] J. Sibik, J. A. Zeitler, 8th International Conference on Broadband Dielectric Spectroscopy and its Applications, September 14-19, 2014 in Wisla, Poland; in press.
[3] M. T. Cicerone, C. L. Soles, Biophys J. **86**, 3836-3845 (2004).

QUANTUM EFFECTS IN THE GLASS TRANSITION AND PROTON CONDUCTIVITY

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Studies of the glass transition usually neglect any quantum effects in structural relaxation. However, our analysis shows [1] that liquids of light molecules with low T_g might have significant contribution of quantum effects. They should lead to a significant decrease of T_g with respect to the melting temperature T_m, and can lead to a sub-Arrhenius temperature dependence of structural relaxation time (instead of usual super-Arrhenius behavior). Combining neutron scattering and dielectric relaxation spectroscopy we show that quantum fluctuations are not negligible in deeply supercooled water and are at the origin of its unusually low fragility, $m \sim 14$ [2]. The discovered anomalously large isotope effect in T_g of water [2] is consistent with the quantum effects dominating structural relaxation of water at these temperatures. It is expected that quantum effects should be strong in proton conductivity because the latter involves motion of the lightest structural unit - proton. Our studies of proton conductivity in phosphoric acids also revealed significant isotope effect. This isotope effect can be ascribed to change in quantum zero-point energy, while no sign of proton tunneling has been found. Thus our studies demonstrate that indeed quantum effects are not negligible for light molecules.

[1] V.N. Novikov and A. Sokolov, Phys. Rev. Lett. **110**, 065701 (2013).

[2] K. Amann-Winkel et al., Proc. Natl. Acad. Sci. USA **111**, 17402-17407 (2014).

THE MECHANICS OF PROTEIN THERMAL STABILITY

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Life is found at both severe cold and hot climates. Extremophilic organisms challenge these extreme environments thanks to their suitable molecular machinery [1]. For example proteins from thermophilic organisms are stable and functional at very high T. How these molecules maintain their folded structures up to the boiling point of water is still unclear and thermal stability is probably the result of a complex balance of disparate molecular factors [2]. Historically, thermal stability has been associated to enhanced mechanical rigidity via the corresponding state principle but recent researches challenged the universality of this paradigm [3].

In this talk we address the issue of the correlation between mechanical and thermal stability in different contexts. We show first that protein mechanical rigidity/flexibility need to be properly defined in term of spatial and temporal length scales pertinent to the molecule, and that the rigid paradigm does not apply to all homologues [4]. Network analysis based on Markov State model is deployed to this aim. We then focus on a specific aspect of mechanical resistance as can be probed by Atomic Force pulling experiments [5]. Preliminary results suggest that weak if not negligible correlation exist among the resistance to the extension driven by external force along the end-to-end distance reaction coordinate and the thermal stability content of the proteins. Finally, we consider how mechanical excitation at level of atomic vibrations scales approaching the melting temperature for proteins under crowding and in different solvents.

All the results of our investigation are based on a computational approach, they will be discussed vis-à-vis of experiments, and the advancing in silico methodology required for the progress of the study will be highlighted.

[1] C. Vieille and G. Zeikus, J. Microbiol. Mol. Biol. Rev. **65**, 1-43 (2001).
[2] F. Sterpone, S. Melchionna, Chem. Soc. Rev. **41**, 1665-1676 (2012).
[3] R. Jaenicke, Proc. Natl. Acad. Sci. U.S.A. **97**, 2962-2964 (2000).
[4] M. Kalimeri, et al., J. Phys. Chem. B **117**, 13775-13785 (2013).
[5] K.M. Tyche et al., Soft Matter **9**, 9016 (2013).

STRUCTURE OF HYDROGENOUS LIQUIDS: SEPARATION OF COHERENT AND INCOHERENT CROSS SECTIONS USING POLARIZED NEUTRONS

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The determination of the coherent structure factor of hydrogenous liquids is very difficult: X-rays are barely sensitive to hydrogen, while neutrons results still lack accuracy due to the contamination of the scattering intensities by a huge spin-incoherent signal from "^{1}H, sometimes reaching over 90% of the measured signal. Theoretical efforts to estimate the incoherent neutron "background" have not yet led to a unique solution, and as a result, the hydrogen bond in e.g. water is still highly debated.

Using polarised neutrons with polarisation analysis, one can experimentally separate the coherent and incoherent contributions to the scattered intensity, since nuclear coherent scattering is purely non-spin-flip, while spin-incoherent scattering is partially (2/3) spin-flip.

We will show the results obtained with this new method on several mixtures of heavy and light water at ambient pressure and temperature: for the first time, we could directly measure the purely incoherent cross section, proportional to the spin-flip scattering, hence allowing an unprecedented accuracy in the extraction of the coherent signal, representative of the structure. On the more theoretical side, we will present recent progress in both the use of Monte Carlo calculations to correct the data for multiple scattering and reverse Monte Carlo calculations, which are shown to properly account for the observed structure factors, also including inelastic contributions (molecular recoil effects).

NEW UNDERSTANDING OF LIQUID THERMODYNAMICS AND SUPERCRITICAL STATE

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Physics textbooks commonly derive and discuss equations for energy and heat capacity for gases and solids but not for liquids. Landau & Lifshitz Statistical Physics textbook states twice that liquid energy can not be calculated in general form, in contrast to solids and gases. The reason for this was summarized by Landau as 'liquids have no small parameter'. Here, based on the old idea of J Frenkel, I formulate the problem in the language of phonons, and calculate liquid energy and heat capacity for both classical and quantum cases. The resulting equation relates heat capacity of the liquid to its relaxation time with no fitting parameters, and is compared with the experimental data of several liquids, including metallic, noble, molecular and network liquids [1].

I subsequently discuss how thermodynamic properties of the liquid change above the critical point using the recent idea that the mean-free path defines the minimal wavelength of longitudinal phonons in the system and our recent finding of the crossover of liquid specific heat in the supercritical state [2].

I finally discuss the new Frenkel line recently proposed to exist in the supercritical state of matter [3,4]. Contrary to the existing view, we have shown that the supercritical state is not physically homogeneous in terms of its properties, but exists in two distinct states: 'rigid' liquids and 'non-rigid' gas-like fluids separated by a dynamic transition across the Frenkel line on the phase diagram. All major properties of the system, including diffusion, viscosity, thermal conductivity, speed of sound and heat capacity as well as structure all undergo qualitative changes at the Frenkel line, from the liquid-like to gas-like [3,4].

[1] D. Bolmatov, V.V. Brazhkin and K. Trachenko, Sci. Rep. **2**, 421 (2012).

[2] D. Bolmatov, V.V. Brazhkin and K. Trachenko, Nat. Comm. **4**, 2331 (2013).

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

[4] V.V. Brazhkin et al., Phys. Rev. E **85**, 031203 (2012); Phys. Rev. Lett. **111**, 145901 (2013).

TRANSVERSE CURRENT SPECTRA OF LIQUID SODIUM: A COMPUTER SIMULATION STUDY

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Quite recently Valentina Giordano and Giulio Monaco [1] have shown that the spectrum of density fluctuations of liquid Sodium, as measured by inelastic X-ray scattering, contains a frequency component which reflects the presence of transverse modes. The argument is confirmed by the parallel measurement of the spectrum of polycrystalline Sodium. The contribution of transverse dynamics to the density-density fluctuation spectrum has long been debated, mostly in connection with molecular and in particular hydrogen bonded systems, but never assumed to be present in simple liquids e.g. liquid alkali metals. Therefore the interpretation of the experimental spectra of liquid Sodium in terms of transverse as well as longitudinal dynamics is a serious challenge to all the previous theoretical understanding based on the projection operator approach. Within this scheme transverse dynamics cannot be explored since longitudinal and transverse currents are mutually orthogonal. In order to confirm (refute) the Giordano-Monaco assumption we have resorted to molecular dynamics calculations of the proper correlation functions, i.e. the longitudinal and transverse currents [2]. We have explored two temperatures, one corresponding to the melting and the other one in a quenched condition corresponding to an amorphous phase. The spectra are analyzed and dispersion curves (omega maximum versus the wavevector k) are reported. A substantial agreement between experimental and computer simulation findings is found.

[1] V. M. Giordano and G. Monaco, Proc. Natl. Acad. Sci. USA **107**, 21985 (2010).

[2] G. De Lorenzi, R. Vallauri, submitted.

GLASSY DYNAMICS ON A SPHERICAL SUBSTRATE

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We study the dynamics of dense assemblies of particles constrained to move on the surface of a sphere, a set-up that is relevant for instance for Pickering emulsions where colloidal particles are confined at the curved interfaces and stabilize the emulsion. Curvature prevents the colloidal system from truly crystallizing at low temperature: irreducible topological defects are always present and thus prevent long-range order. At low temperature, these defects tend to form complex structures, called 'grain boundary scars', which are observed experimentally. The dynamics of such colloidal assemblies has received so far little attention and we investigate the problem through Molecular Dynamics simulations. The relaxation is found to become very slow as temperature decreases, and the system acquires the properties of a glassy state. We study the characteristics of this glassy dynamics in detail as a function of the radius of the sphere. We complement the numerical investigation by a description of the glassy freezing via an extension of the equations of mode coupling theory (MCT) for liquids on the surface of a sphere.

T-REX: A TIME-OF-FLIGHT RECIPROCAL SPACE EXPLORER FOR THE FUTURE ESS SOURCE

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We present the proposal of a time-of-flight chopper spectrometer for the future ESS neutron source. The instrument is designed to yield a dynamic range that extends from 20 μeV to 150 meV in energy transfer and from 0.01 Å^{-1} to 17 Å^{-1} in wavevector transfer. The elastic energy resolution (FWHM) can be freely adjusted in the range from 1% to 3% at 3 meV and from 4% to 8% at 100 meV.

T-REX has been benchmarked against existing state-of-the-art neutron TOF-spectrometers and shows flux gain factors between one and two orders of magnitude and possible solutions are foreseen to increase the signal to noise ratio. These features make the instrument a real game changer in a manifold of scientific research activities: magnetism, strongly correlated electron materials, functional materials, soft-matter, biophysics and disordered systems.

It will implement time-of-flight spectroscopy with Polarization Analysis as a standard tool, e.g. to uniquely derive the vibrational hydrogen excitations in soft matter through separation of the nuclear spin incoherent scattering. Moreover, thanks to the high flux, T-REX is clearly an excellent tool to investigate small samples (sub 100 mg) and the identification of small signals: nowadays both these characteristics are at the forefront of the neutron research in soft-matter.

The wide energy transfer range available enables studies of picosecond diffusional and relaxational dynamics of biosystems as well as their vibrational counterpart, in one experiment, while keeping the sample under controlled environmental conditions. Parametric studies (e.g. variable T or P) of the vibrational density of state will become routine, while the polychromatic character of T-REX (Repetition Rate Multiplication) will open new ways for studies of vibrations characterized by damped phonon-like excitations in disordered systems.

THE UNIMPRESSIVE ORIGIN OF THE APPARENT FRAGILE-STRONG TRANSITION

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Supercooled water is suspected to undergo a fragile-strong transition (FST). Theoretical interest has been fostered by a possible connection with a Widom line emanating from the phase boundary between low and high density amorphous ice. Experimental support for the FST has mostly come from high-resolution neutron spectroscopy. The FST appears as a kink in the temperature dependence of a mean relaxation time $\langle\tau\rangle$. This interpretation depends critically on the assumption that the experiment sees one and the same relaxation process above and below the kink. Based on new backscattering spectra of water in carbon nanohorns we show that the contrary is the case.

Formally, our fit function is the same as regularly used in support of a FST: a sum of a delta line, accounting for elastic scattering by the matrix, and a Kohlrausch spectrum. This model suffers from parameter degeneracies. Occam's razor tells us to maximize constraints under minimal physical assumptions. We use harmonic extrapolations of the T dependent scattering intensity to fix the amplitudes in our delta-plus-Kohlrausch fits. We then identify two q, T regions that admit particularly stringent constraints, and a crossover regime in between. In this way, we find that quasielastic scattering reveals different physics in different q, T regimes: At low T, it is dominated by localized motion; at high T by relaxation-coupled diffusion.

Mapping the structure of a glass through its voids

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Positron annihilation lifetime spectroscopy is employed to measure the size of the interstitial void spaces characterizing the structure of a set of permanently densified SiO_2 glasses. The average volume of the voids is markedly affected by the densification process and linearly shrinks by almost an order of magnitude after a relative density variation of 22%. In addition, x-ray diffraction shows that this change of density does not modify appreciably the short range order, which remains organized in SiO_4 tetrahedra. These results strongly suggest a porous medium description for v-SiO_2 glasses where the compressibility and the medium range order are dominated by the density variation of the voids volume up to densities close to that of α-quartz.

Part III

Posters

LINK OVERLAP FLUCTUATIONS IN SPIN GLASSES

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The critical behavior and the diagrammatic structure of spin glasses in zero field are the object of several studies. Some physical observables have not been explored in detail near the critical point, arousing our interest in filling these gaps and exhibiting appropriate theoretical models for propagators. In analogy with the linear operator Q_{ab} which identifies the overlap matrix in field theory, we approach the problem in the RS phase for quadratic operators $Q_{ab}\ Q_{cd}$ in order to find out three orthonormal and independent subspaces and extrapolate their anomalous dimensions. By developing a perturbative expansion in $D = 6-\epsilon$ with a cubic replica symmetric invariant, we focus our attention on 1PI diagrams both in a scalar theory and in a generic cubic theory involving a third rank tensor. The latter method provides the characteristic functions of RG according to the MS scheme and hence the leading critical exponents, with particular attention to that associated with the specific heat. The second eigenvalue resulting from the quadratic operator diagonalization might be related to a new weakly divergent quantity known in literature as "link-overlap susceptibility", for which a different dependence with respect to the energy fluctuations arises.
Finally, borrowing de Almeida-Thouless terminology for linear operators, we analyse the most relevant scaling laws in the limit $n \to 0$, highlighting a degeneracy between anomalous and longitudinal sectors which causes logarithmic corrections.

EFFECTS OF CLAY CONTENT ON THE PROPERTIES OF POLYSACCHARIDE-BASED HYDROGELS

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Hydrogels are three dimensional networks capable of absorbing large amounts of water while maintaining their dimensional stability. The integrity in their swollen state can be maintained by physical and/or chemical crosslinking. In chemically crosslinked hydrogels, the linear polymer chains are covalently bonded with each other via crosslinking agents whereas physically crosslinked hydrogels are usually spontaneously formed by weak secondary forces. The introduction of physical crosslinks to the chemical network led to hydrogels that exhibit improved mechanical properties. One strategy to create chemical and physical crosslinks simultaneously is to introduce into the chemical network hydrogen bonding with clay nanofillers. In this work, the influence of different amounts of montmorillonite (MMT) on the structural and rheological properties of polysaccharide based hydrogels was investigated. Depending on the clay content, different nanostructures were identified by X-ray diffraction (XRD) and their effect on the rheological properties of the dual hydrogels was studied. The reaction mechanism between the polysaccharide, the filler and the crosslinking reagent was examined by using FTIR-ATR spectroscopy. The observed blue and red shifts of some characteristic functional groups suggested the hydrogen bonding is the principal mechanism of interaction. The XRD results confirmed that the property improvements were related to the MMT exfoliation and good interaction between the polysaccharide blend and MMT. Dynamic stress and frequency sweep tests evidenced that the presence of different composite nanostructures influences differently the rheological behavior of the investigated system. On the basis of the obtained results, a model structure was proposed according to which the clay sheets act as effective multifunctional cross-linkers.

Vibrational imaging: a non-invasive investigation of living cells

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Cellular imaging techniques have become powerful tools in cell biology. With respect to others, the techniques based on vibrational spectroscopy present a clear advantage: both the molecular composition and the modi?cation of subcellular compartments can be obtained in label-free conditions. In fact, from the evolution of positions, intensities and line widths of Raman and infrared bands in the cell spectra, characteristic information on cellular structures can be achieved. We present the time evolution of the Raman spectra of single live Jurkat cells (T-lymphocyte) [1] and SHSY5Y cells (human neuroblastoma cells) growth also on memristive surface [2]. The investigation of methylene vibrations, markers of cellular membrane fatty acids [3], can represent an important method to study and to monitor the state of the cellular membrane and its alteration as consequence of diseases, inflammation, hypoxia and different stages of cellular death. The data behavior presented here, independently from the investigated cell line, represents the proof-of-concept for this approach showing the potential of the proposed marker. The experimental procedure we used, together with the analysis of these high frequency vibrational bands, may be considered a new, complementary and advantageous technique to investigate on cellular biology and physiology.

[1] S.Caponi et al. J. Biophys. Chem. **152** 58 (2013).

[2] Research ongoing in a multi-/inter-disciplinary project named MaDEleNA funded by the Provincia

Autonoma di Trento "Grandi Progetti 2012".
[2] P. Sassi et al. J. Raman spectroscopy, submitted

LOW TEMPERATURE HEAT CAPACITY OF COMPACTED SiO_2 GLASSES

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A study of low temperature specific heat capacity (1-30 K) and low frequency Raman scattering (6-200 cm^{-1}) has been performed on SiO_2 glasses, which have been compacted under pressures up to 8 GPa to explore different glassy phases having growing density. Increasing densification by more than 20% leads to a progressive reduction of the specific heat capacity C (more than a factor 4) and to a shift from 10 K up to about 17 K of the broad peak observed above 1 K in a C/T^3 vs. T plot. It has been also revealed a parallel and progressive decrease of the intensity of the Boson peak observed in the Raman spectra, whose frequency BP increases from about 50 cm^{-1} in v-SiO_2 up to more than 90 cm^{-1} in the most compacted glass. The variations of the calorimetric peak temperature Tpeak are stronger than those experienced by the elastic Debye temperature Θ_D, implying changes of the low-energy vibrational dynamics which are not accounted for by the transformations of the elastic continuum. By using the low-frequency Raman intensity to determine the temperature dependence of the low temperature heat capacity, it has been assessed the density of low-frequency vibrational states $g(\nu)$. The observations performed over SiO_2 compacted glasses are compared to the predictions of theoretical models and computer simulations explaining the nature of the Boson peak. Consistency with the results of a simulation study concerning the vibrations of jammed particles leads to evaluate a nanometer length scale which suggests the existence of poorly packed domains.

DYNAMICS OF ANHYDRO-RING BASED SUGAR AND ITS AQUEOUS MIXTURES STUDIED BY BROADBAND DIELECTRIC SPECTROSCOPY

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The present study deals with dynamic and thermodynamic properties of 1,6-Anhydro-glucose, known also as levoglucosan (LG) in comparison with those of glucose (G) [1].

The structure of LG differs from that of G for an insertion of the oxygen bridge between two carbons into the pyranose ring, that results strained by the formation of the anhydro-ring. The more rigid and stable ring avoids the muta-rotation process in LG, contrary to G. Moreover, due to its compact form, LG molecules may show, in addition to the crystalline and supercooled liquid state, a transition to plastic crystal form, absent in G [2]. Also intermolecular and intramolecular interactions are strongly different. LG has less hydroxyl groups for ring than G, nevertheless the formation of hydrogen bonding is still quite strong, assured by O-H...O intermolecular bonds [3,4]. Dynamics of LG have been studied using dielectric spectroscopy and numeric simulations [1]: the blocking of the hydroxyl-methyl unit suppresses the intramolecular γ-secondary relaxation active for G and makes α-relaxation more sensitive to temperature. On the other hand, thanks to the lower number of OH groups, α-relaxation is faster. On mixing LG with water, the dynamics of water in the mixture result much more affected than in the case of G, on considering similar molar concentration, in agreement with recent studies [5].

[1] K. Kaminski et al, J. Phys. Chem. B **114**, 11272 (2010).

[2] F. Shafizadeh et al., Carbohydr. Res. **13**, 184 (1970).

[3] M. Sladkovicova et al., J. Mol. Struct. **874**, 108 (2008).

[4] L. Smrcok et al., Acta Cryst. B **62**, 912 (2006).

[4] S. Corezzi et al., J. Chem. Phys. **140**, 184505 (2014).

From the microscopic to collective dynamics in aqueous solutions of a thermoresponsive microgel

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The thermosensitivity of poly(N-isopropylacrylamide) (PNIPAM) microgels, related to the competition between hydrophobicity and hydrogen bonding, has made these particles especially popular in the field of drug release, chemical separation, and surface modification, and as a model for protein denaturation as well. We have studied the thermal behavior of PNIPAM microgel particles with two different sizes and different concentrations in water, by means of photo-correlation (PCS), Brillouin (BLS) and infrared (IR) spectroscopy, in order to investigate how the volume phase-transition correlates with variations of collective properties (i.e. sound waves at GHz frequencies, probed by BLS) and variations of single particle structural properties (i.e. changes in conformation, interaction, and microenvironment of individual chemical groups, probed by IR). From the viewpoint of collective vibrations, the phase transition of microgel particles does not greatly affect the velocity of acoustic waves in the medium, but dramatically affects their attenuation. Surprisingly, the impact on the acoustic properties seems to be characterized by two different regimes, at lower and higher concentrations. From the viewpoint of single particle, as probed by variations in the band profile of chemical groups interacting with water, detected in the middle-IR region, we observe that C=O groups of swollen particles are mainly involved in hydrogen bonding (C=O H-N or C=O H-O) and then, in collapsed particles the fraction of free C=O groups increases. On the other hand, variations of the band profile characteristic of bulk water, detected in the near-IR region, probe the transition from the viewpoint of solvent medium. It is found that water signals are identical in the presence or absence of swollen particles, indicating that interstitial water is similar to bulk water. Interestingly, when particles are collapsed the fraction of free OH groups increases, indicating that hydration water is less bonded than bulk water.

MELTING LINE INVARIANTS OF THE LENNARD-JONES SYSTEM

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In this work we studied the invariance of some properties of the well-known Lennard-Jones (LJ) system along the melting line. These properties have already been widely studied in the past. The reason to further investigate this subject is related to the attempt to explain why these invariances hold. In our view these invariances are a consequence of isomorphs theory and we give prof of this hypothesis using computer simulations.

We prove first that the melting line for LJ system can be approximated with high accuracy by an isomorph, melting isomorph; then we show that the invariances observed on the melting isomorph, are also observed on other isomorphs in the liquid and crystalline phase. More specifically, we studied the behaviour of structure structure, mean square displacement and bulk shear viscosity. The interest in studying these properties is related to the possibility of spreading light on why some known melting criteria holds (Hansen-Verlet criteria and Lindemann criteria) and why Andrade equation give a good estimation of melting viscosity for liquid metals.

Our conclusion is that all these empirical observations can be explained by isomorph theory and that they are not peculiarities of the melting line but they holds on every isomorph.

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

[2] T.B. Schrøder et al., J. Chem. Phys. **134**, 164505 (2011)

[3] L. Separdar et al., J. Chem. Phys. **138**, 154505 (2013)

SYNTHESIS OF HYDROGEN CLATHRATE HYDRATE FROM LIQUID PHASE

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The nucleation and growth from the liquid phase of a solid clathrate-hydrate is a process even less understood and more difficult to study compared to that of a pure liquid. By means of in situ Raman spectroscopy, we have examined this phenomenon for the system hydrogen and water, which exhibits a stable solid clathrate phase in the range of pressure 1-2 kbar and temperature 273-263 K. Our sample is initially a liquid solution of hydrogen in water in contact with pressurized hydrogen gas at 2 kbar and at a temperature of about 264 K (i. e. outside the stability region of common ice Ih). After about 10 hours, we start to detect the vibrational spectrum of caged hydrogen molecules (well distinguished from that of H_2 in solution) which increases in intensity while the solid clathrate grows. From the analysis of the Raman intensity, we can infer the population of the small (512) and large (51264) cages as a function of time during the hydrogen clathrate growth. Its behaviour, observed here for the first time, has some analogies with what observed in the more studied case of methane hydrate, where the small 512 cages play a key role in the first stage of nucleation. However, the possibility for H_2 of multiple occupation of the large cages introduces an extra degree of freedom for the determination of the hydrate stoichiometry.

REVIEW OF LATTICED DYNAMICS AND LATTICE THERMAL CONDUCTIVITY OF SKUTTERUDITES

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The skutterudite structured crystalline solids are cage like in the sense that they contain both occupied and unoccupied large microscopic cubic volumes associated with a simple cubic sublattice of transition metal atoms. It has been discovered experimentally that the room temperature thermal conductivity is much lower (factor of 5 or 10) for synthesized so-called filled skutterudites (nominally ternary compounds such as $LaCoFe_3Sb_{12}$) than the comparable unfilled ones (binary compounds such as $CoSb_3$). There has been much recent interest in explaining this observation due to the requirement of low lattice thermal conductivity for good thermoelectrics of which the materials with skutterudite structures have promise as they also tend to have large Seebeck coefficients.

Various lattice dynamics studies including filling atom dynamics and direct relaxation time based and Green Kubo based approaches to calculating thermal conductivity will be covered. In particular, it seems to be the consensus of recent literature that a highly anharmonic filling atom dynamics suggested by the well-known rattling ion concept is inconsistent with first principles based calculations. In addition, these latter calculations appear to provide explanations of lower thermal conductivity in terms of differences in host atom interactions, both harmonic and anharmonic, and in terms of ordinary cubic anharmonic interactions between the filling atom and the neighboring host atoms. We consider work done on a barium filled antimonide skutterudite in addition to the above mentioned lanthanum filled one.

WATER STRUCTURE IN AQUEOUS DISPERSIONS OF SILVER NANOPARTICLES

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Water is the most common compound all over the world and a vital part of every leaving organism. Raman spectroscopy is very useful technique in studies of water structure and molecular interactions in complex systems of liquid water [1]. Silver nanoparticles (AgNPs) are gaining popularity in industrial applications [2], hence it is very important to investigate their influence on water structure and interactions between them. In Raman spectrum of water dispersions of AgNPs in OH stretching vibration region we observe enhancement of band around 320 cm^{-1}, assigned to locally-structurised water, in comparison to pure water spectrum. This suggests organization of water molecules near to AgNPs. Results of Raman investigations on water dispersions of AgNPs synthesized by simple chemical reduction [3] will be presented. The AgNPs thermo- and photostability will be also discussed.

This work was financially supported from grant no. 2013/09/B/ST4/03010.

[1] N.A. Chumaevskii and M.N. Rodznikova, J. Molecular Liquids **109**, 2433-2441 (2011).

[2] S.J. Oldenburg and A.E. Saunders, Material Matter **9**, 64-67 (2014).

[3] A.J. Frank et al., J. Chem. Education **87**, 1098-1101 (2010).

NEW INSIGHTS ON THE SPECIFIC HEAT OF GLASSES

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The physical properties of disordered systems are currently in the focus of a large research effort. In particular, one of the open problems related to glasses is their excess of modes over the vibrational contribution predicted by the Debye model. In fact, one could expect the continuum approximation underlying the Debye model to hold in glasses at long wavelengths at least as well as in crystalline solids. The experiments, instead, show that the specific heat at low temperature (a few Kelvin) and the density of vibrational states at low frequency (a few terahertz) are very different from the Debye prediction. We present here a detailed analysis of specific heat measurements of vitreous GeO_2, a prototype of strong glasses, and of permanently densified vitreous GeO_2. Our data give experimental evidence that glasses do not show any excess of vibrational modes when compared to their crystalline counterparts of similar mass density. The presence of an excess of states over the Debye model appears to be a mere consequence of the inadequacy of the Debye approximation at terahertz frequencies.

PREDICTION OF DYNAMIC FRAGILITY FROM THERMODYNAMIC PARAMETERS

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The concept of fragility is currently of interest in the research fields such as formulation of amorphous drug and food preservation, because it is considering as a key factor which correlates with the glass-forming ability and physical stability of the amorphous systems. This is because the parameter m is related to an average degree of molecular mobility reflected in structural relaxation τ_α near the glass transition. The molecular mobility in *fragile* glass formers varies rapidly with temperature near the glass transition temperature T_g in contrast to that occurring in *strong* liquids. This difference has been considered to be the reason to expect that strong liquids are more physically stable than fragile liquids. The fragility manifests not only kinetically in the temperature dependence of $\log \tau_\alpha$ (as the degree of its departure from the Arrhenius behavior), but also in the thermal response of glass-formers. A lot of effort has been put into predicting the parameter m using only calorimetric methods. In this presentation, we test several models of thermodynamic fragility [1–3] for various amorphous drugs and verify their correlations with the dynamic fragility established on the basis of dielectric measurements.

[1] K.A. Graeser et al., Eur. J. Pharm. Sci. **37**, 492–498 (2009).
[2] J.A. Baird, B. Van Eerdenbrugh, L.S. Taylor, J. Pharm. Sci. **99**, 3787 (2010).
[3] K.J. Crowley and G. Zografi, Thermochim. Acta **380**, 79–93 (2001).

MONTE CARLO SIMULATION OF OH–RADICALS REACTION KINETICS IN WATER ENVIRONMENT WITH RADICAL SCAVENGERS

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Hydrogels and polymer networks in general, should be considered as systems with very high complexity. It has been shown that efficient method of obtaining polymer networks, commonly with water as solvent phase, is pulse radiolysis (e.g. [1,2]), where the reactions involving pulse-induced radicals are essential. The detailed mechanism and kinetics of radiation-induced reactions of different polymers in aqueous solution still remain not fully explored. We proposed the use of Monte Carlo simulation with diffusion and explicit shown solvent molecules – the Dynamic Lattice Liquid (DLL) model [3]. This model bases on the assumption that diffusion steps are realized as cooperative motion. Pure radical system was taken as a test case. Reaction kinetics for different fraction of low-molecular-weight radical scavengers with various mobility and reaction rate constant were analyzed. Radicals concentration reflected high dilution (c.a. 50 ppm) to model experimental conditions obtained with use of typical linac system. Results were compared with analytical solution and classical Monte Carlo kinetic simulation. Radicals decay time was also considered in the case were radical scavengers had a form of linear polymer chains with different length.

[1] P. Ulanski, Zainuddin, J.M. Rosiak, Radiat. Phys. Chem. **46**, 913 (1995).
[2] J.K. Jeszka, S. Kadlubowski, P. Ulanski, Macromolecules **39**, 857 (2006).
[3] J. Saramak et al., J. Mol. Model. **20**, 2529 (2014).

THE ATTRACTIVE INTERACTIONS BETWEEN LIKE IONS AND HYDROPHOBIC INTERACTIONS IN WATER LIQUID, AND POSITRON AND ION MIGRATIONS IN THE LIQUIDS

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The investigation for ion mobility in the liquid phase has been one of the central area of physical chemistry. The electrohydrodynamic theory by Habbard and Onsager [1] and the stockastic theory for ionic conductivity in the liquid phase have been proposed. Since fluctuation from the equilibrium medium is preferable in liquid phase, localization of ions such as positrons is highly probable. Gramsh et al. [2,3] have observed very different behaviour of the diffusion length $L+$ of positrons in liquid and solid metals. Kanazawa and coworkers[4-6] proposed a qualitative explanation for the increase of the positron diffusion length $L+$ with temperature in the liquid phase. In addition,Kanazawa and coworkers [7,8] have suggested one origin of the attractive interaction between like ions in liquids. In this study, we have analyzed in more detail the positron diffusions in the liquid metals, and have discussed the field theoretical formula of like ions attractive interactions and hydrophobic interaction in water liquid and the relation to the Hubbard-Onsager dielectric theory.

[1] J. Hubbard and L. Onsager, J. Chem. Phys. **67**, 4865 (1977).
[2] E. Gramsh, K.G. Lynn, J. Throwe, I. Kanazawa, Phys. Rev. Lett. **67**, 1282 (1991).
[3] E. Gramsh, K.G. Lynn, J. Throwe, I. Kanazawa, Phys. Rev. B **59**, 14282 (1999).
[4] I. Kanazawa, Radial. Phys. Chem. **58**, 457(2000).
[5] Y. Matsushita, H. Kitahata, I. Kanazawa, Phy. Stat. Sol. (c) **4**, 3546(2007).
[6] H. Kitahata, Y. Matsushita, I. Kanazawa, Appl. Surf. Sci. **244**, 167 (2008).
[7] I. Kanazawa, H. Suzuki, H. Kitahata, J. Phys. CS **225**, 012024 (2010).
[8] K. Yamada, M. Saito, H. Suzuki, I. Kanazawa, Mater. Sci. Forum **733**, 132 (2013).

RANDOM-WALK SIMULATION OF PROTONIC DEFECT DYNAMICS IN DOPED ICE

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Water molecules can condense into a wide variety of crystalline phases of which 16 are currently known to exist. However, more phases are predicted or discussed to exist at ambient or elevated pressures. Motivated by a large number of experimental results demonstrating that the enhancement in proton dynamics occurs differently for different dopants and in different ice phases, and with an interest to study defect-induced mobility as a function of doping concentration, we carried out random walk simulations for different types of dopants in different ice structures. Several aspects addressed in this context are how and at which doping concentration the mobility of a certain defect is affected by the presence of other defects or by their path within the ice lattice. The latter issue is particularly important for dynamics and referred to in literature as "path blocking": a diffusion pathway (or a part thereof) taken by a defect becomes unavailable for the passage of another defect of the same type.

We thank K. Amann-Winkel, V. Fuentes-Landete, T. Loerting and B. Geil for providing us with ice samples and for the stimulating discussions. Support of this project by the Deutsche Forschungsgemeinschaft, Grant No. BO1301/12-1, is gratefully acknowledged.

ROSKILDE UNIVERSITY MOLECULAR DYNAMICS WITH GPUS

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We present a molecular dynamics framework designed and optimized for running on graphics processing units.

CONDUCTIVITY AND DIELECTRIC RELAXATION IN LIQUID AND SUPERCOOLED LIQUID $PYR_{1,4}TFSI$ DOPED WITH LI TFSI

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Ionic liquids are largely considered as promising electrolytes to be used in new batteries and technological devices related to energy storage and exploitation of renewable energy sources. The addition of Li salt to pure ionic liquids has been proposed as a way to improve the electrochemical stability, with only little decrease of their ionic conductivity at room temperature. Along with dc conductivity, another important parameter for applications of ionic liquids is their dielectric permittivity. As revealed by broadband dielectric spectroscopy experiments, the frequency dependent behavior of the complex permittivity for ionic liquids is similar to the dielectric relaxation exhibited by dipolar molecular liquids. In this work we have studied the broadband dielectric response of $(\mathrm{Li\ TFSI})_x(\mathrm{PYR}_{1,4}\ \mathrm{TFSI})_{1-x}$ mixtures, with $x = 0, 0.05, 0.10, 0.20$, in the frequency range between 100 mHz and 3 GHz, aiming at clarifying the influence of Li-salt doping on the dielectric relaxation of the ionic materials, both in the liquid and supercooled liquid temperature range. The results have been analyzed also in terms of the complex electric modulus and complex frequency dependent conductivity. A comparison with current models for the dynamical response of ion conducting materials has been carried out.

[1] A. Matic and B. Scrosati, MRS Bull. **38**, 533-537 (2013).
[2] A. Martinelli et al., J. Phys. Chem. B **113** 11247-11251 (2009).

CONDUCTIVITY ENHANCEMENT, DIELECTRIC RELAXATION, AND NON ARRHENIUS TRENDS IN OCTANOIC ACID / BIS(2-ETHYLHEXYL) AMINE BINARY MIXTURES

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Binary mixtures of the amphiphilic materials octanoic acid and bis(2-ethylhexyl) amine, have been investigated by broadband dielectric spectroscopy as a function of temperature. Depending on the composition, the dc conductivity of the mixture is several orders of magnitude higher than that of the pure components at room temperature. The higher the conductivity of the mixture, the lower is the relaxation frequency at which the dielectric relaxation occurs. Moreover, non Arrhenius trends of the dc conductivity and of the dielectric relaxation time vs. temperature have been observed for some of the mixtures above their melting temperature. The formation of transient eteroadducts of OA and BEEA molecules, most likely 2(OA):BEEA, could be responsible for the conductivity enhancement versus composition, as well as for the increase of the viscosity, and for the slowing down of the dielectric relaxation. This picture, supported by the results of Wide Angle X rays Scattering and 1H-NMR measurements, can also account for the peculiar temperature dependence of the dc conductivity and of the dielectric relaxation.

[1] P. Calandra et al., J. Mat. Chem C, accepted.
[2] P. Calandra et al., J. Chem. Phys. **136**, 064515 (2012).
[3] P. Calandra et al., J. Coll. Interf. Sci. **367**, 280 (2012).

NONLINEAR XY AND P-CLOCK MODELS ON SPARSE RANDOM GRAPHS: MODE-LOCKING TRANSITION OF LOCALIZED WAVES

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A statistical mechanic study of the XY model with nonlinear interaction is presented on bipartite sparse random graphs. The model properties are compared to those of the p-clock model, in which the planar continuous spins are discretized into p values. We test the goodness of the discrete approximation to the XY spins to be used in numerical computations and simulations and its limits of convergence in given, p-dependent, temperature regimes. The models are applied to describe the mode-locking transition of the phases of light-modes in lasers at the critical lasing threshold. A frequency is assigned to each variable node and function nodes implement a frequency matching condition. A non-trivial unmagnetized phase-locking occurs at the phase transition, where the frequency dependence of the phases turns out to be linear in a broad range of frequencies, as in standard mode-locking multimode lasers at the optical power threshold.

MOLECULAR INSIGHT INTO IBUPROFEN SODIUM SALT SIGNIFICANCE FOR VOLUME PHASE TRANSITION IN POLYMER-WATER-DRUG SYSTEM

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The main area of presented research includes investigations of an influence of ibuprofen sodium salts on Volume Phase Transition Temperature (T_{VPT}) of poly(2-(2-methoxyethoxy)ethyl methacrylate) ($PMEO_2MA$) hydrogels. This polymer is commonly regarded as a good candidate for biomedical applications because of its biocompability and non-toxicity [1]. The reasons of this unique behavior will be discussed in the light of spectroscopic results. Raman spectroscopy was used to characterize the specific intermolecular interaction between water-polymer networks and ibuprofen sodium salt [2].

This project was supported by Polish National Science Center (grant no. 2013/09/B/ST4/03010) and Young Scientists' Fund at the Faculty of Chemistry, Technical University of Lodz.

[1] J.F. Lutz, Adv. Mater. **23**, 2237-2243 (2011).

[2] M.N. Olejniczak, K. Piechocki, M. Kozanecki, K. Koynov, A. Adamus, R.A. Wach, unpublished materials.

ISOMORPHS IN SYSTEMS WITH NON-ISOMOPHIC DEGREES OF FREEDOM

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The isomorph theory predicts that for a large class of liquid systems, structure and dynamics - as well as certain thermodynamic properties - are invariant along the same lines in the density-temperature phase diagram [1]. Isomorphs can be found in several way, for instance from fluctuations in potential energy and virial. Isomorphs have been found by MD simulations in atomic systems as well as for different kinds of stiff molecules, e.g. flexible chains [2] and experimental evidence of isomorphs has also been established [3].

So far it has not been possible to predict isomorphic state points in molecular systems with intra molecular springs, despite the fact that state points with the correct scaling behavior have been found empirically. The problem seems to be the vibrational degrees of freedom which contributes to the instantaneous potential energy and virial.

With a combination of NVT MD and Monte Carlo simulations and using free energy differences we integrate out the vibrational DOFs at fixed non-vibrational DOFs. By studying a simple dumbbell model with intra molecular springs, this procedure allows us to find state points that have the same structure and dynamic, uncovering a new class of pseudo isomorphic systems that obey the isomorphic predictions for a subset of their DOFs.

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

[2] A.A. Veldhorst et al., J. Chem. Phys **141**, 054904 (2014)

[3] L. Bøhling et al., New Jour. Phys. **14**, 113035 (2012).

MICROSCOPIC DYNAMICS IN THE GLASS FORMER B_2O_3 MEASURED BY X-RAY PHOTON CORRELATION

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Despite the strong efforts carried out over the last decades, a microscopic description of the glassy state is still missing. One of the main obstacles to advance in the field arises from the difficulty of achieving information on the dynamics at the atomic scale. Here we exploit the unique characteristics offered by X-ray photon correlation to directly observe the dynamics at the microscopic length-scale in the strong glass former B_2O_3. In the supercooled liquid phase, the microscopic dynamics is more than a decade faster than that measured with macroscopic techniques, as already observed in other systems. Surprisingly, instead, the microscopic dynamics is not frozen in the glassy state: it remains of the order of 100 s, with slight temperature dependence below the glass transition.

OPTOMECHANICAL CHARACTERIZATION OF SUB-MICRON SIZED GLASSES

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A novel approach to broadband picosecond acoustics (BPA), which enables to determine simultaneously the elastic modulus and the refractive index dispersion in the visible range, has been developed to study ultrastable glasses prepared by (PVD) physical vapor deposition. BPA is a pump probe experiment based on generation and detection of coherent vibrational excitations. It is a time domain version of Brillouin scattering, which can be perfomed on submicron thick materials as PVD. Our glassy samples are coated with a thin metallic film which absorbes the infrared pump pulse and instantaneously thermally expands launching a longitudinal acoustic wave packet inside the overlying material. The travelling density fluctuaction is probed by a second delayed broadband pulse monitoring the differential reflectivity as function of its time delay. Each probe wavelength λ couples to a phonon of defined wave vector $Q(\lambda)$, visualized as oscillations of reflectivity whose frequency ω depends sound velocity, refractive index and the angle of incidence β. By determining the transient reflectivity maps for different scattering geometry, hence angles β, both sound velocity v and refractive index at each λ can be inferred. Remarkably, the refractive index dispersion proved to be in excellent agreement with ellipsometry data. This approach can be extended to a extremelly large class of material with disomogeneities on few hundred nm scale and unknown optomechanical properties.

SHORT-RANGE ORDER OF COMPRESSED AMORPHOUS $GeSe_2$

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Amorphous materials have played a significant role in the last decades both from the technological point of view that on pure research grounds. Applications such as phase-change memory storage and infrared lenses are being investigated to gain insight into the physical processes governing the phenomena and to optimize the devices efficiency. The recently developed temperature-dependent constraint theory helps identify the ideal composition in order to get the best mechanical and rheological properties of glass materials. Nevertheless, a heated debate concerning the presence of an 'intermediate phase' or of wrong (homopolar) bonds is still open. In this work we present a structural analysis performed onto amorphous $GeSe_2$ under pressure (up to 30 GPa) by means of double-edge X-ray absorption spectroscopy. The topological modifications induced by pressure in the short-range structure around the photo-absorbers have been characterized by looking at the first-shell radius and its mean square disorder σ_0^2. The possibility of 'sitting' separately on the two atomic species has given us a way to virtually extend the energy range available and therefore better refine the structural parameters. In particular, the analysis of the ambient conditions spectra suggests the presence of chemical disorder for about 20%. Upon compression, we observed an elongation of the Ge-Se tetrahedral distance compatible with an increase in the coordination number, accompained by a metallization process.

DPPC Diffusion in Alcoholic Environment

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The effects of butanol and octanol on the phase behavior and on the lateral mobility of 1,2-palmitoyl-sn-glycero-3-phosphocholine (DPPC) have been studied by performing differential scanning calorimetry (DSC) and pulsed-gradient stimulated-echo (PGSTE) NMR measurements. Both liquid and interdigitated phases have been investigated. A lowering of the lipid transition from the gel to the liquid crystalline state for the membrane?alcohol systems has been observed. NMR measurements reveal three distinct diffusions in the DPPC-alcohol systems, characterized by a high, intermediate, and slow diffusivity, ascribed to the water, the alcohol, and the lipid, respectively. In the liquid phase the lipid diffusion process is promoted by the presence of both butanol and octanol, while in the interdigitated phase it is hindered by the presence of alcohols. Furthermore, in the interdigitated phase, lipid lateral diffusion coefficients show a slight temperature dependence. By the Arrhenius plots of the temperature dependence of the diffusion coefficients, the apparent activation energy in both the liquid and the interdigitated phase have been evaluated. The presence of alcohol increases this value in both phases. An explanation in terms of a two dimension free volume model that takes into account for both the free area available for diffusion and the activation energy of the diffusion process for energy factors is proposed.

THE STRUCTURE FACTOR OF LIQUID PROPANOL BY POLARIZED NEUTRON DIFFRACTION

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Alcohols are important compounds widely used as solvents and many of their particular properties are due to the existence of intermolecular hydrogen bonds. The structure of the liquid phase of the lowest members of the series has been determined by neutron diffraction, such as methanol, ethanol and iso-propanol. The signature of H-bonded molecular association in diffraction data is the formation of a pre-peak at a scattering vector, $Q \approx 0.7 - 0.8$ Å^{-1}, before the main diffraction peak. The pre-peaks of liquid alcohols,

which are well known in X-ray diffraction data, have been detected in the neutron diffraction pattern only recently. The neutron scattering technique is sensitive to the positions of both the C and H nuclei.
The extremely high value of the incoherent neutron cross-section of hydrogen and its exiguous coherent scattering would make it impossible to extract from the total signal the contribution of the partial correlations. For this reason, we determined the structure factor of liquid propanol using polarized hot neutrons on D3. Measuring the spin-flip and non-spin-flip contributions, we are able to directly measure the incoherent scattering cross section and subtract it from the total scattering. This technique allows us removing an important proportion of the incoherent 'background' and obtaining the structure factor with high precision. For comparison purposes, we also conducted experiments on deuterated propanol, for which the incoherent contribution is less important.

A molecular dynamics study of a 2D system of hard ellipses

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We have simulated the dynamics of a two dimensional system of hard ellipses by event-oriented molecular dynamics in NEV ensemble. Various quantities namely longitudinal and transverse velocity auto-correlation functions, translational and rotational diffusion mean squared displacements, pressure, intermediate self scattering function, radial distribution function and angular spatial correlation have been obtained and their dependence on packing fraction is characterized. Despite absence of prominent positional ordering, the orientational degree of freedom behaves nontrivially and exhibits interesting features. Slowing down is observed in the angular part of the motion near isotropic-nematic phase transition. It is shown that above a certain packing fraction the rotational mean squared displacement exhibits a three stage temporal regime including a plateau. Comparison to 2D system of hard needles is made and it is shown that from positional viewpoint, the ellipse system is more ordered.

Diffusivity of water molecules in hydrogel matrixes

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Stimuli responsive polymer hydrogels which can exhibit volume phase transition (VPT) are a new generation of materials with many applications such as micro-valves, chemical indicators, drug delivery systems, lenses and many others [1,2]. The rapidness of VPT (crucial for most of mentioned applications) depends mainly on molecular relaxations of polymer network stressed in fully swallen state as well as on the mobility of water molecules [3]. Thus, it is extremely important to know the water diffusivity in such complex systems. Currently, the time and spatial resolution offered by experimental techniques allows only to observe averaged picture of diffusive properties of water in complex systems. In this work the results of Monte Carlo simulations (DLL model [4]) for aquaoues solutions of polymer chains and simple stars (modeled the crosslinkage in hydrogel) in athermal case are considered. Influence of polymer chain lenghts, and concentration on water diffusivity is discussed. The water mobilility in various distances from polymer chain is shown. This project was supported by Polish National Science Centre (grant no. 2013/09/B/ST4/03010).

[1] Y. Li et al, Chem. Soc. Rev. 41, 2193 (2012).
[2] M. Pastorczak, PhD thesis, Lodz University of Technology (2010).
[3] T. Tanaka and D.J. Fillmore, J. Chem. Phys. 70 1214 (1979).
[4] J Saramak et al., J. Mol. Model. 20, 2529 (2014).

TERAHERTZ-INDUCED CRYSTALLIZATION OF AMORPHOUS SYSTEMS

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Terahertz radiation excites inter-molecular vibrational (librational) response in amorphous systems, represented in the vibrational density of states (VDOS). Upon crystallization of an amorphous sample VDOS collapses to a limited number of phonon modes. With the advancement of free-electron laser sources the generation of extremely powerful terahertz pulses has become possible. Using the FLARE beam line at the FELIX Laboratory in Nijmegen, The Netherlands, we performed first experimental studies on inducing crystallization in amorphous systems with intense terahertz radiation. The FLARE beam consists of trains of micro pulses (length of 10-100 ps). Each train forms a macro pulse of about 10 μs length. The peak power in the micro pulse is at the order of 10^5 Watt. Such a terahertz beam provides enough energy to disturb the inter-molecular hydrogen-bonded network and to induce crystallization in amorphous carbamazepine, indomethacin and paracetamol. Particular care was given to exclude the role of sample heating in the crystallization process under the FLARE beam. Crystallization was induced in amorphous carbamazepine with active cooling of the sample even at 258 K (-15°C), far below its glass transition temperature, $T_g = 325$ K. The amorphous systems studied under intense terahertz radiation crystallized into different polymorphs than those typically obtained by sample heating.

INFERENCE FOR INTERACTING LINEAR WAVES IN ORDERED AND RANDOM MEDIA

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A statistical inference method is developed and tested for pairwise interacting systems whose degrees of freedom are continuous angular variables, such as planar spins in magnetic systems or wave phases in optics and acoustics. We investigate systems with both deterministic and quenched disordered couplings on two extreme topologies: complete and sparse graphs. To match further applications in optics also complex couplings and external fields are considered and general inference formulas are derived for real and imaginary parts of Hermitian coupling matrices from real and imaginary parts of complex correlation functions. The whole procedure is, eventually, tested on numerically generated correlation functions and local magnetizations by means of Monte Carlo simulations.

SUPERDIFFUSION AND TRANSPORT PROPERTIES IN SYSTEMS WITH LÉVY LIKE QUENCHED DISORDER

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Lévy-like motions are an important family of random motions, generated by a stochastic process with stationary and independent increments of arbitrary length l featuring a heavy tail $l^{-(a+b)}$ where d is the space dimension.

An experimental situation where Lévy motion can be detected is diffusion in heterogeneous and porous media such as the recently developed Lévy-Glass, an optical system with quenched disorder and a tunable power-law distribution of the scattering length. In this work we characterize this system in two dimensions by developing a poly-modal sphere random close packing algorithm, performing simulations on the undergoing dynamics and measuring the transport properties and the scaling of the dynamical quantities with the system size. We present a thorough characterization of the packing efficiency, revealing the parameters driving the filling fraction behavior and in what conditions the latter does not behave as expected in a fractal system. We then simulate the dynamics, finding a strong correlation between the filling fraction behavior and the dynamical observables. In

particular, keeping the filling fraction constant or trying to maximize it at every system's size reflects in observing two different classes of dynamical properties.
The different behavior of the system reveals the leading role played by the filling fraction and underlines the necessity to develop a consistent packing algorithm in future studies of the system.

T-REX: A TIME-OF-FLIGHT RECIPROCAL SPACE EXPLORER FOR THE FUTURE ESS SOURCE

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We present the proposal of a time-of-flight chopper spectrometer for the future ESS neutron source. The instrument is designed to yield a dynamic range that extends from 20 μeV to 150 meV in energy transfer and from 0.01 Å^{-1} to 17 Å^{-1} in wavevector transfer. The elastic energy resolution (FWHM) can be freely adjusted in the range from 1% to 3% at 3 meV and from 4% to 8% at 100 meV.
T-REX has been benchmarked against existing state-of-the-art neutron TOF-spectrometers and shows flux gain factors between one and two orders of magnitude and possible solutions are foreseen to increase the signal to noise ratio. These features make the instrument a real game changer in a manifold of scientific research activities: magnetism, strongly correlated electron materials, functional materials, soft-matter, biophysics and disordered systems.
It will implement time-of-flight spectroscopy with Polarization Analysis as a standard tool, e.g. to uniquely derive the vibrational hydrogen excitations in soft matter through separation of the nuclear spin incoherent scattering. Moreover, thanks to the high flux, T-REX is clearly an excellent tool to investigate small samples (sub 100 mg) and the identification of small signals: nowadays both these characteristics are at the forefront of the neutron research in soft-matter.
The wide energy transfer range available enables studies of picosecond diffusional and relaxational dynamics of biosystems as well as their vibrational counterpart, in one experiment, while keeping the sample under controlled environmental conditions. Parametric studies (e.g. variable T or P) of the vibrational density of state will become routine, while the polychromatic character of T-REX (Repetition Rate Multiplication) will open new ways for studies of vibrations characterized by damped phonon-like excitations in disordered systems.

COLLECTIVE ION DYNAMICS IN LIQUID ZINC: EVIDENCE FOR COMPLEX DYNAMICS IN NON-FREE ELECTRON LIQUID METAL

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We present a detailed inelastic neutron scattering investigation of the THz dynamics of liquid zinc. The observed Q-dependence clearly reveals the existence of a complex dynamics made up of two distinct excitations. The highest energy mode is the prolongation of the longitudinal acoustic density fluctuations whereas the comparison with the phonon dynamics of crystalline *hcp* zinc suggests a transverse acoustic-like nature for the second one. This mode seems related to peculiar anisotropic interactions, possibly connected to the anomalous behavior of the crystalline phase.

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