Workshop on Soft Matter
Self Assembly and Dynamics

Information and Abstract Book

January 9 – 10, 2014

Hyderabad, India

Tata Institute of Fundamental Research
Centre for Interdisciplinary Sciences
Hyderabad

UNIVERSITY OF HYDERABAD
हैदराबाद विश्वविद्यालय

Contents

Organization

The workshop is jointly organized by TIFR Centre for Interdisciplinary Sciences (TCIS), TIFR and University of Hyderabad (UoH).

Conveners

Surajit Dhara, V S S Sastry (University of Hyderabad)
Narayanan Menon, Srikanth Sastry (TIFR Centre for Interdisciplinary Sciences, Hyderabad)

Contact Information

Please contact Ms. Roopa (TCIS) if you need any assistance or have any questions. You may also contact the other people listed here if necessary.

Name	**Telephone Nos.**	
Ms. Roopa	+91 40 2419 5117	+91 98860 89777
Surajit Dhara		+91 97012 40875
Narayanan Menon		+91 88863 60132
Srikanth Sastry		+91 94483 86838
TCIS Reception	+91 40 2419 5001	
Guest House, UoH	+91 40 2313 2150	
TCIS Hostel / Guest House enquiry	+91 40 2419 5001	
Security TCIS Hyderabad	+91 40 2419 5208	

Transport during workshop

UoH Guest House to C R Rao Centre	8.40 AM
C R Rao Centre to UoH Guest House	5.45 PM
Aparna Sarovar (TCIS Guest House), Aparna Cyber (TCIS Student Hostel), Magadha Village, TCIS to C R Rao Centre	Will be Arranged (to and fro)

Programme of Workshop on Soft Matter : Self Assembly and Dynamics
January 9 – 10, 2014, TCIS, Hyderabad, India

Day 1 : Thursday, January 9 2014

Time	Lecturer	Lecture Topic
9:00 – 9:30	Pick up Conference material and welcome session	
9:30 - 10:00	C. Austen Angell	Structural transitions in metallic and semiconducting glassformers: some phenomenological relationships with connections to phase change switching materials
10:00 - 10:30	Upadrasta Ramamurty	Fracture in amorphous alloys
10:30 - 11:00	**COFFEE BREAK**	
11:00 - 11:30	Peter H. Poole	Heterogeneous nucleation in the low-barrier regime
11:30 - 12:00	Sarika Bhattacharyya	Interplay between crystallization and glass transition
12:00 - 12:30	Surajit Sengupta	The crystal road to glass: Non-affine droplet fluctuations in crystalline solids
12:30 - 14:00	**LUNCH BREAK**	
14:00 - 14:30	Jeppe Dyre	What distinguishes a complex system from a simple?
14:30 - 15:00	Chandan Dasgupta	Beta relaxation in glass-forming liquids from dynamics in a (meta)basin
15:00 - 15:30	Shankar P Das	Localization, disorder and boson peak in an amorphous solid
15:30- 16:00	**COFFEE BREAK**	
16:00 - 16:30	Debasish Chaudhuri	Stochastic pump of interacting particles
16:30 - 17:00	Shankar Ghosh	Super-spreading of charged granular matter
17:00 - 17:30	Sanat K Kumar	Glass Transitions in Polymer/Nanoparticle Composites

Day 2 : Friday, January 10 2014

Time	Lecturer	Lecture Topic
9:00 - 9:30	Smarajit Karmakar	Static Length Scale in Glass Transition
9:30 - 10:00	Francesco Sciortino	Simple models of competitive interactions in soft-matter:re-entrant liquids and gels on heating
10:00 - 10:30	Pinaki Chaudhuri	Rheology of soft jammed particles: role of attractive interactions
10:30 - 11:00	**COFFEE BREAK**	
11:00 - 11:30	Cristiane Alba-Simionesco	Self-organisation and miscibility limit in molecular hydrogen bonded liquids
11:30 - 12:00	Charusita Chakravarty	Triplet Correlations in Tetrahedral Liquids
12:00 - 12:30	P Viswanath	Specific ion effects at interfaces
12:30 - 14:00	**LUNCH BREAK**	
14:00 - 14:30	Himanshu Khandelia	Packing Parameter Matching of Cholesterol with Oxidized Phospholipid Species in Lipid Bilayers
14:30 - 15:00	Gilles Tarjus	Fluids and solids at curved interfaces
15:00 - 15:30	Slobodan Zumer	Knotted nematic fields: recent developments
15:30- 16:00	**COFFEE BREAK**	
16:00 - 16:30	P B Sunil Kumar	Nematogens on membranes : Aggregation and morphological changes.
16:30 - 17:00	M Krishnan	Low-energy structural relaxations and the onset of anharmonic diffusive dynamics in proteins
17:00 - 17:30	KPN Murthy	Kinetic Walks and Compact Polymer Conformations

Lecture abstracts

Structural transitions in metallic and semiconducting glassformers: some phenomenological relationships with connections to phase change switching materials

C. Austen Angell

Arizona State University

Email: austenangell@gmail.com

Abstract:

One of the more surprising developments in the area of metallic glassformers in recent years has been the suggestion by Zhang et al (J.Chem. Phys. 133, 014508 (2010) that a large number of metallic glassformers exhibit some sort of structural transition, manifested as a change from fragile liquid character at high temperature to strong liquid character at lower temperature approaching the glass transition. This occurs in the temperature range where the crystallization is particularly rapid, and the two are no doubt closely related. This sort of behavior was previously considered a characteristic only of certain highly anomalous "tetrahedral liquids" like water, and liquid silicon. In the latter, the transition is also a metal-to-semiconductor transition as suggested long ago by Turnbull and coworkers for Si and Ge, before confirmation by the simulations of Grabow, Sastry and their coworkers.

In the metallic glassformer case, of course, the transition cannot be assigned to any electron localization phenomenon, while in the water case, there is no hint of delocalized electrons, so we must search for some more general explanation. We note that in the cited cases, the glass transition occurs below the liquid-liquid phase transition, where the liquid exhibits "strong" liquid characteristics. Analogous behavior is seen in the case of the strong extreme of rotator phase crystals, where the high temperature limit is a lambda transition of theoretically well-understood character. In liquids, lacking crystalline order, the lambda form is only observed at a particular pressure, where it is a critical point terminating a line of first order liquid-liquid transitions. At different pressures the density fluctuations may be damped out before becoming critical, or may be preempted by a first order transition. We illustrate these features using "potential tuning" MD of the Stillinger-Weber model for liquid silicon. Finally, we link these ideas to known density anomalies (with supercritical appearance) in supercooled liquid Te, and stable liquid As2Te3, and discuss how they might find practical manifestation in the fast switching phenomena of "phase change" materials (which contain these two elements and Ge in similar proportions).

(Angell, in Physics and Applications of Disordered Materials (Honoring Stan Ovshinsky on his 80th: editor M. Popescu) pp 1-18 (2002)).

Fracture in amorphous alloys

Upadrasta Ramamurty

Indian Institute of Science, Bangalore

Email: ramu@materials.iisc.ernet.in

Abstract:

The mechanical properties of amorphous alloys have proven both scientifically unique and of potential practical interest, although the underlying deformation and fracture physics in them remain less firmly established as compared with crystalline alloys. In this presentation, I shall review the recent advances we made in understanding the fracture behaviour of metallic glasses. In crystalline metals and alloys, the term 'ductile' is synonymous with 'tough,' as they both are linearly correlated. However, the non-existence of such correlation in metallic glasses poses a conundrum. For example, bulk metallic glasses (BMGs) with no tensile ductility whatsoever can exhibit extraordinarily high fracture initiation toughness values. "What is the physical reason for such high toughness?" is a question that we set out to answer. A related issue is the following: A material physics-based condition, at which fracture will initiate, is essential for reliable design of components and structures. Fracture criteria for brittle materials like ceramics are stress based whereas those in ductile materials like metals and alloys are strain based. But, both need the identification of a critical length scale, l*, which is related to some microstructural length scale, to be prescribed *apriori.* A suitable fracture criterion is needed to identify l* at which plastic to brittle transition takes place. Mixed-mode fracture experiments coupled with detailed finite element simulations are conducted identify the fracture criterion in a nominally ductile BMG. These results show that fracture in amorphous alloys is controlled by the attainment of a critical strain and that a stable crack grows inside a shear band at the notch root before attaining criticality at l*≈60 µm. The Argon and Salama model, which is based on meniscus instability phenomenon at the notch root, has been modified to rationalize the physics behind this length scale. This model suggests that the mean ridge heights on fractured surfaces were found be correlated to the toughness of the BMG. In contrast, the fracture mechanism in brittle metallic glasses is elusive. Some interesting morphologies observed on brittle fracture surfaces will be presented.

Heterogeneous nucleation in the low-barrier regime

Peter H. Poole

St. F Xavier University, Canada

Email: ppoole@stfx.ca

Abstract:

In simulations of the two-dimensional Ising model, we examine heterogeneous nucleation induced by a small impurity consisting of a line of l fixed spins. As l increases, we identify a limit of stability beyond which the metastable phase is not defined. We evaluate the free energy barrier for nucleation of the stable phase and show that, contrary to expectation, the barrier does not vanish on approach to the limit of stability. We also demonstrate that our values for the height of the barrier yield predictions for the nucleation time (from transition state theory)and the size of the critical cluster (from the nucleation theorem) that are in excellent agreement with direct measurements, even near the limit of stability.

Interplay between crystallization and glass transition

Sarika Bhattacharyya

NCL, Pune, India

Email: mb.sarika@ncl.res.in

Abstract:

In this talk I will discuss the interplay between crystallization and glass transition in different binary mixtures by changing their inter-species interaction length and also the composition. We find that only those systems which form bcc crystal in the equimolar mixture and whose global structure for larger xA (xA = 0.6, where xA is the mole fraction of the bigger particles) is a mixed fcc + bcc phase, do not crystallize at this higher composition. However, the systems whose equimolar structure is a variant of fcc (NaCl type crystal) and whose global structure at larger xA is a mixed NaCl + fcc phase, crystallize easily to this mixed structure. We find that the stability against crystallization of this “bcc zone” is due to the frustration between the locally preferred structure (LPS) and the mixed bcc + fcc crystal. Our study suggests that when the global structure is a mixed crystal where a single species contributes to both the crystal forms and where the two crystal forms have large difference in some order parameter related to that species then this induces frustration between the LPS and the global structure. This frustration makes the systems good glass former. When xA is further increased (0.70< xA < 0.90) the systems show a tendency towards mixed fcc crystal formation. However, the “bcc zone” even for this higher composition is found to be sitting at the bottom of a V shaped phase diagram formed by two different variants of the fcc crystal structure, leading to its stability against crystallization.

The crystal road to glass: Non-affine droplet fluctuations in crystalline solids

Surajit Sengupta

TIFR Centre for Interdisciplinary Sciences, Hyderabad

Email: surajit@tifrh.res.in

Abstract:

A crystalline solid exhibits thermally induced localised non-affine droplets in the absence of an external stress. Upon an imposed shear, the size of these droplets grow until they percolate at a critical strain well below the value at which the solid begins to yield. This critical point does not manifest in bulk thermodynamic or mechanical properties, but is hidden and reveals itself in the onset of inhomogeneities in elastic moduli, disappearance of a metastable liquid-glass spinodal and sudden enhancement in defect pair nucleation with associated structural and dynamical consequences. Introducing a field which couples to non-affine displacements in crystals, enhances non-affine fluctuations and stabilizes the, ordinarily metastable, glassy minima causing a thermodynamic, crystal to glass transition. Many of our results such as single point and two point spatial and temporal correlation functions of non-affine fluctuations and the phase boundary for the crystal to glass transition may be obtained semi-analytically.

What distinguishes a complex system from a simple?

Jeppe Dyre

Roskilde University, Denmark

Email: dyre@ruc.dk

Abstract:

Many systems in soft matter have intriguing and complex phase diagrams. This applies even for the apparently simple model defined by the radially symmetric Gaussian core potential. This example shows that it is not just the existence of multiple time and length scales that makes a system complex, thought in practice this is often the case. We here argue that simple systems are those with an (approximate) hidden scale invariance [1], and that complex systems are those without such. Hidden scale invariance refers to the property that a change of density merely leads to a linear (affine) transformation of the potential energy surface. This property implies the existence of isomorphs, which are curves in the thermodynamic phase diagram along which structure and dynamics are invariant in properly reduced units [2]. It also implies a separation of the equation of state such that temperature is the product of a function of density and a function of excess entropy.

References :

1. J. C. Dyre, Phys. Rev. E 88, 042139 (2013).
2. N. Gnan et al, J. Chem. Phys. 131, 234504 (2009).

Beta relaxation in glass-forming liquids from dynamics in a (meta)basin

Chandan Dasgupta

Indian Institute of Science, Bangalore

Email: cdgupta@physics.iisc.ernet.in

Abstract:

To be announced

Localization, disorder and boson peak in an amorphous solid

Shankar P Das

Jawaharlal Nehru University, New Delhi

Email: shankar0359@yahoo.com

Abstract:

The inhomogeneous density n(x) of a solid, often treated as an order parameter in the density functional theories (DFT), is usually expressed as a sum of gaussian profiles respectively centered around the different points of a lattice $\{R_i\}$. The average width of the gaussian profiles represents a characteristic length ℓ signifying the degree of mass localization in the system. Using analysis based on entropic considerations, we show here that as ℓ for anamorphous solid spreads beyond a critical value ℓ_0, the corresponding vibrational density of states $g(\omega)$ deviates from the Debye form $g_D(\omega)$ to develop the boson peak. For a hard core system of diameter σ we obtain $\ell_0 = 0.2\sigma$.

Stochastic pump of interacting particles

Debasish Chaudhuri

IIT Hyderabad

Email: debc@iith.ac.in

Abstract:

We consider overall directed motion of repulsively interacting Brownian particles under the influence of unbiased pumping forces that vanish under spatial or temporal averaging. For one dimensional motion analytic results are obtained, showing particle-hole symmetry, and current reversal with changing density.

For two-dimensional colloids under a flashing ratchet drive, molecular dynamics simulations reveal a different density dependence of current from the results obtained in one dimension, and the resonance frequency show a non-monotonic variation with density. We use mean field arguments to describe these results. We further show how the change in dynamic behavior is associated with structural transformation in the colloidal dispersion.

Super-spreading of charged granular matter

Shankar Ghosh

TIFR, Mumbai

Email: sghosh@mailhost.tifr.res.in

Abstract:

I will speak on the vertical spreading of a monolayer of glass particles on a plastic (polypropylene/polystyrene) surface driven by an orbital shaker. The interactions in the system evolve in time through the progressive triboelectric charging of the surfaces involved. The particles spread initially through splashing and sticking onto the cylinder's surface forming an amorphous monolayer. Continued driving initiates a collective motion, i.e., 'super spreading', of this monolayer, first forming wavy stripes - spatially periodic density modulations, and then ejecting narrow particle jets, hundreds-of-particle-diameter-long and few diameters wide, from the tips of the stripes. The jets eventually coalesce laterally to form a homogeneous spreading front, layered along the spreading direction. This remarkable growth patterns are related to the spatially inhomogeneous and temporally intermittent frictional drag between the moving charged glass particles and the much-less-mobile counter-charges on the plastic container.

Glass Transitions in Polymer/Nanoparticle Composites

Sanat K Kumar

Columbia University, New York, USA

Email: sk2794@columbia.edu

Abstract:

The role of surfaces on the glass transition temperature of small molecule and polymeric fluids has been a topic of considerable interest in the last two+ decades. Inspite of this ongoing interest the field has remained controversial. A few experimental results have suggested that surfaces can significantly affect the Tg, while newer results suggest that surfaces play a minor role in this context. Similar, confusing results have also been found from simulations. We use detailed computer simulations and show that there should only be small effects when polymers are confined between strongly attractive surfaces. The essentially irreversible adsorption of polymer chains to a nanoparticle effectively modifies the boundary condition experienced by a polymer melt – so that the bulk polymer "sees" itself. Under these situations there should be minimal changes in Tg and in the fragility, results that seem to be more prevalent in the newer body of experimental literature. The consequences of these findings on the role of nanoparticles on the reinforcement of a polymer's mechanical properties are also discussed.

With D. Meng, F. Starr, J. Douglas.

Static Length Scale in Glass Transition

Smarajit Karmakar

TIFR Centre for Interdisciplinary Sciences, Hyderabad

Email: smarajit@tifrh.res.in

Abstract:

Glasses are liquids whose viscosity has increased so much that they cannot flow. Accordingly there have been many attempts to define a static length-scale associated with the dramatic slowing down of supercooled liquid with decreasing temperature. In this talk, I will present a simple method to extract the desired length-scale which is highly accessible both for experiments and for numerical simulations. The fundamental new idea is that low lying vibrational frequencies come in two types, those related to elastic response and those determined by plastic instabilities. The minimal observed frequency is determined by one or the other, crossing at a typical length-scale which is growing with the approach of the glass transition. This length-scale characterizes the correlated disorder in the system: on longer length-scales the details of the disorder become irrelevant, dominated by the Debye model of elastic modes. After introducing the length-scale I will show how this scale completely determines the dynamics of the supercooled liquid under external constraints, thereby proving beyond doubt the static nature of the proposed length-scale. Then I will try to explain how this length scale can be used to explain all the finite size effects seen in simulations of glass forming liquids and its possible universal relation with the relaxation time. Finally I will try to establish the possible relation between this length scales and other proposed length scales like point to set length scale and patch length scale etc.

Simple models of competitive interactions in soft-matter:re-entrant liquids and gels on heating

Francesco Sciortino

Roma La Sapienza, Italy

Email: francesco.sciortino@uniroma1.it

Abstract:

I will discuss how unconventional phase diagrams can arise in extreme cases of colloids interacting with competing interactions. Specifically I will discuss the case of dipolar hard spheres, where self-assembly into chains compute with the phase separation process and the case of a patchy particle model that behaves similarly. Then I will discuss how this concept of competing interactions can be exploited to design a system that gels on heating. Finally I will suggest a possible experimental realisation based on DNA nano-constructs.

References:

Lorenzo Rovigatti, Jose´ Maria Tavares, and Francesco Sciortino, Self-Assembly in Chains, Rings, and Branches: A Single Component System with Two Critical Points, Phys.Rev.Lett. 111, 168302 (2013)
Sandalo Roldan-Vargas, Frank Smallenburg, Walter Kob and Francesco Sciortino, Gelling by heating Scientific Report 3, 2451 (2013)
Silvia Biffi et al, Phase behavior and critical activated dynamics of limited-valence DNA nano stars, Proceedings National Academy of Science, 110 15633-15637 (2013).

Rheology of soft jammed particles: role of attractive interactions

Pinaki Chaudhuri

University of Dusseldorf

Email: pinaki@thphy.uni-duesseldorf.de

Abstract:

In nature, soft disordered solids occur in different forms (eg. gels, emulsions, colloids, foams, grains etc) across a wide range of packing fractions, which is made possible by the tuning of particle interactions. The flow properties of these soft materials have been harnessed for various applications in our daily lives. Thus, understanding the role of particle interactions and the corresponding mechanisms which lead to observed rheological behaviour is an important recurrent theme.

Using numerical simulations, we study the rheological response of an athermal assembly of soft particles with tunable attractive interactions, in the vicinity of jamming. At small attractions, a fragile solid develops and a finite yield stress is measured. Moreover, the measured flow curves have unstable regimes, which lead to persistent shear-banding. These features are rationalized by establishing a link between the rheology and the number of contacts per particle, which also provides a minimal model to describe the measured flow curves.

Self-organisation and miscibility limit in molecular hydrogen bonded liquids

A.Raihane1, C. Crauste-Thibierge1, P-A. Artola2 , B. Rousseau2, D. Morineau3, C. Alba-Simionesco1
(1) Laboratoire Léon Brillouin ,CNRS /CEA -UMR 12, CEA Saclay, 91191 Gif-sur-Yvette Cedex, France
(2) Laboratoire de Chimie-Physique ,CNRS -UMR 8000, Univ. Paris Sud Bât. 349 , 91405 Orsay Cedex France
(3) Institute of Physics of Rennes, CNRS-University of Rennes 1, France

Cristiane Alba-Simionesco

CEA, Paris, France

Email: christiane.alba-simionesco@cea.fr

Abstract:

We focus on molecular liquids that spontaneously form supramolecular clusters and on their consequences on the dynamical properties in the supercooled liquid state. We study a particular class of glass-forming liquids, mono-alcohols, where the molecular self-association driven by the presence of H-bonds is counterbalanced by the steric hindrance of the alkyl chains. We focus on an archetypical one, ter-butanol and analyze the mesoscopic structures and length-scales observed in binary mixtures, either with water on one side or with an aprotic solvent. Neutron and X-rays scattering, are combined with viscosity and dielectric experiments and supported by MD simulations.

Triplet Correlations in Tetrahedral Liquids

Charusita Chakravarty

IIT, Delhi

Email: charus@chemistry.iitd.ernet.in

Abstract:

The total, triplet and pair contributions to the entropy with increasing tetrahedrality are mapped out for the Stillinger-Weber liquids to demonstrate the qualitative and quantitative differences between triplet-dominated, tetrahedral liquids and pairdominated, simple liquids with regard to supercooling and crystallization. We show that as a function of tetrahedrality, the liquid state can be subdivided into pair- and tripletdominated regimes, separated by a narrow, glass-forming region where orientational disorder within the first neighbour shell is significant. The three regimes show qualitatively different thermodynamic behaviour on supercooling, with the lowtetrahedrality liquids conforming to the temperature scaling and melting rules expected of simple liquids, while the triplet-dominated systems show a characteristic heat capacity anomaly reflecting local ordering due to pair and triplet correlations prior to crystallization. The results suggest that structural correlations can be directly related to thermodynamic anomalies, phase changes and self-assembly in other atomic and colloidal fluids.

References:

1. M. Singh, D. Dhabal, A. H. Nguyen, V. Molinero, and C. Chakravarty, Triplet Correlations Dominate the Transition from Simple to Tetrahedral Liquids (submitted).
2. D. Nayar, B. S. Jabes, D. Dhabal, S. Gangopadhyay, S. Prasad and C. Chakravarty, Structural Correlations and Onset of the Density Anomaly in Tetrahedral Liquids (in preparation).

Specific ion effects at interfaces

P Viswanath

Centre for Soft Matter Research, Jalahalli, Bangalore – 560 013

Email: viswanath@csmr.res.in

Abstract:

Ions have profound impact on very many physico-chemical and biological processes. In 1888, Franz Hofmeister has classified the ions based on its effectiveness towards 'salting in' or 'salting out' of proteins from aqueous solutions [1]. The sequence for anions and cations are: Cl- > NO3- > Br- > ClO4- ~ SCN- and Cs+ < Rb+ < NH4+ < K+ < Na+ < Li+ < Ca2+ < Mg2+ < Zn2+, respectively. Such a sequence is also found to be applicable to properties like surface tension, surface potential and viscosity of aqueous salt solution, foam stability, cloud point temperature, micellar growth, enzyme activity, aggregation of amyloid fibrils and phase sequence in lyotropic liquid crystals [2]. In some cases, the sequence is also found to be reversed and depends on salt concentration [3].

Classical electrostatics fail to describe these puzzling behavior even for ions with same valency. Several refinements were introduced taking into account the ion size, valency, polarizability, hydration characteristics, chemical (direct ion binding) and solvent interactions to explain the specific ion effects in the literature [4]. The salt and the solvent effects at interfaces is also known to play a major role [5]. Our efforts towards understanding the role of ions at air-aqueous electrolyte, lipid-electrolyte and liquid crystal-aqueous electrolyte interfaces will also be discussed.

References:

1) Zur Lehre von der Wirkung der Salze' (about the science of the effect of salts): Franz Hofmeister's historical papers, W. Kunz et al. Current Opinion in Colloid & Interface Science, 9 (1–2), 19 (2004).
2) Specific ion effects, Ed. W. Kunz, World Scientific, Singapore (2010).
3) M. Bostrom et al. Langmuir, 27, 9504 (2011); Zhang, Y. and Cremer, P.S. PNAS, 106 (36), 15249 (2009).
4) Koelsch et al. Coll. and Surf. A: Physicochem. and Engg. Asp. 303 (1–2), 110 (2007).
5) Cacace MG et al. Q. Rev Biophys. 30, 241 (1997).

Packing Parameter Matching of Cholesterol with Oxidized Phospholipid Species in Lipid Bilayers

Himanshu Khandelia

MEMPHYS, Center for BioMembrane Physics, University of Southern Denmark SA (SDU)

Email: hkhandel@sdu.dk

Abstract:

We claim that (1) cholesterol protects bilayers from disruption caused by lipid oxidation by sequestering conical shaped oxidized lipid species such as 1-palmitoyl-2-azelaoyl-sn-glycero-3-phosphocholine (PZPC) away from phospholipid, because cholesterol and the oxidized lipid have complementary shapes and not because cholesterol orders lipid bilayers and (2) mixtures of cholesterol and oxidized lipids can self-assemble into bilayers much like lysolipid– cholesterol mixtures. The evidence for bilayer protection comes from molecular dynamics (MD) simulations and dynamic light scattering (DLS) measurements. In simulations, bilayers containing high amounts of PZPC become porous, unless cholesterol is also present. The evidence for the pairing of cholesterol and PZPC comes mainly from correlated 2-D density and thickness plots from simulations, which show that these two molecules co-localize in bilayers. Further evidence that the two molecules can cohabitate comes from self-assembly simulations, where we show that cholesterol- oxidized lipid mixtures can form lamellar phases at specific concentrations, reminiscent of lysolipid–cholesterol mixtures. The additivity of the packing parameters of cholesterol and PZPC explains their cohabitation in a planar bilayer. Our hypothesis has important consequences for cellular cholesterol trafficking; diseases related to oxidized lipids, and to biophysical studies of phase behaviour of cholesterol-containing phospholipid mixtures.

Fluids and solids at curved interfaces

Gilles Tarjus

LPTMC, Université Pierre et Marie Curie, Paris, France

Email: tarjus@lptl.jussieu.fr

Abstract:

To be announced

Knotted nematic fields: recent developments

Slobodan Zumer

University of Ljubljana and Jozef Stefan Institute

Email: slobodan.zumer@fmf.uni-lj.si

Abstract:

High geometrical constrains and intrinsic chirality may lead to stable and metastable knotted nematic fields. Recently it was demonstrated that knots and links of arbitrary complexity can be formed with laser micro-manipulation of nematic braids of -1/2 disclinations entangling colloidal particles. Understanding stability, ordering, and assembly of such topological soft matter systems requires a synergy of theoretical, simulation, and experimental approaches. In this overview of our recent achievements I first describe an extension of the conventional topological description of nematic defects by including the self-linking number as a topological invariant useful in classifying nematic disclination networks. This approach is then illustrated with four numerically modeled nematic braids: i) knotted 2D nematic colloidal crystals, ii) 3D opal structures permeated by nematics, iii) knots in cholesteric droplets, and iv) mutually tangled colloidal knots and defect loops in nematic fields.

Nematogens on membranes: Aggregation and morphological changes.

P B Sunil Kumar

IIT Madras

Email: sunil@iitm.ac.in

Abstract:

The organelles of a biological cell have membranes with highly curved edges and tubes, as seen in the endoplasmic reticulum, the golgi and the inner membrane of mitochondria. It has been shown that macromolecules, which constitute and decorate the membrane surface, strongly influence the morphology of membranes. The standard Helfrich model for membranes, based on mean curvature energy, cannot explain the stability of such highly curved structures. Existence of anisotropic bending energy, which could arise from an in-plane orientational field on the membrane, will be the minimal requirement to explain the stability of such shapes. Planar orientational order could be intrinsic to the membrane, due to the structural properties of its constituents, or could arise as a result of membrane interactions with external agents.

We use a numerical model of the membrane, with elongated membrane inclusions possessing spontaneous directional curvatures that could be different along, and perpendicular to, the membrane's long axis. We show that, due to membrane-mediated interactions, these curvature inducing membrane-nematogens can aggregate spontaneously, even at low concentrations, and change the local shape of the membrane.

Energy Landscape and Fast Side Chain Dynamics of Proteins

M Krishnan

IIIT, Hyderabad

Email: m.krishnan@iiit.ac.in

Abstract:

Fast side chain conformational dynamics play an important role in the biological function of proteins. High-resolution solution NMR spectroscopy uses side chain methyl spin probes to determine the amplitudes and rates of site-specific fast internal motions of proteins. In particular, the methyl axial order parameter (O2), which quantifies the spatial restriction of side chain motion, is commonly used to establish a molecular-level connection between the atomistic dynamics and thermodynamics of proteins.

We have examined the connection between the topography of the underlying energy landscape and the fast side chain conformational dynamics of proteins using molecular dynamics simulations and enhanced sampling free energy methods. The side chain conformational free energy surfaces obtained using the adaptive biasing force (ABF) method for a set of eight proteins with different molecular weights and secondary structures reveal universal features of fast side chain motions in proteins.

Kinetic Walks and Compact Polymer Conformations

K.P.N. Murthy

School of Physics, University of Hyderabad

Email: kpnmsp@uohyd.ernet.in

Abstract:

I shall talk about self avoiding walks (SAW) that model polymer conformations. The athermal SAW becomes thermal, when we introduce non-bonded nearest neighbour contact interactions. We call this an Interacting Self Avoiding Walk(ISAW). Employing blind ant algorithms we can generate an ensemble of polymer conformations. By attaching Boltzmann weights we can calculate canonical ensemble averages of desired properties.

We can think of myopic ant algorithms that reduce attrition; but then we have to carry extra weights, called Rosenbuth-Rosenbluth(RR) weights to get averages right. These RR weights fluctuate and PERM algorithms address the problems that arise from these fluctuations.

We can interpret a myopic ant as generating Kinetic Growth Walk (KGW) - a walk that grows faster than it equilibrates. In this talk I shall consider a variant Interacting Growth Walk (IGW) that helps generate compact conformations useful in the study of low temperature behaviour of linear homopolymer. I shall also talk of calculating the entropy of Interacting Self Avoiding Walks from growth models.

How to reach the University of Hyderabad?

At the main gate, enquire for the directions to the Jubilee Guest House for accommodations. The workshop will be held at the auditorium of the C.R.Rao Advanced Institute of Mathematics, Statistics and Computer Science (AIMSCS).

From RGI Airport

The University is 35 km from the Shamshabad Airport and can be reached by taxi (MERU tel: 44224422; or Easy cabs tel: 43434343) or by the bus operated by GMR. The Taxi charges approximately Rs: 600/- whereas by bus Rs.200/-. You need to get down at Gachibowli and travel another 4 km by auto to reach the University. The University Guest House is about 1 Km from main gate.

From Railway Station

Hyderabad (Nampally) : 20 Km to the campus
Secunderabad : 30 Km to the campus
Kacheguda : 28 Km to the campus
Lingampally : 4 Km to the campus

Metro rail operates to Lingampally from all other stations at regular intervals

From the Bus Station

Mahatma Gandhi Bus Station (Earlier know as Imliban): 26 Km to the campus