**Symposium on “Contemporary Issues in Condensed Matter Systems”**  
**June 13-15, 2016**

Venue: Indian Institute of Science, Bangalore  
Organized By: Department of Physics IISc Bangalore  
Organizing Committee Chairman:  
Prof. V. Venkataraman, Dept of Physics, IISc Bangalore 560012  
Tel: +91 80 2293 2314 or +91 80 2293 3286 Mob: 98867-98515  
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Final Technical Program:

**June 13th Monday (Venue: Faculty Hall, IISc)**

<table>
<thead>
<tr>
<th>Time</th>
<th>Event</th>
</tr>
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<tbody>
<tr>
<td>9.15 - 9.30 AM</td>
<td><strong>Inaugural Function</strong></td>
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<tr>
<td>9.30 - 10.20 AM</td>
<td>Inaugural Lecture by Prof. C.N. R. Rao, JNCASR Bangalore</td>
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<tr>
<td>10.20 - 10.40 AM</td>
<td>Tea / Coffee break</td>
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<tr>
<td>10.40 - 11.20 AM</td>
<td>Technical Session: I (Chaired by Prof. K.S. Narayan)</td>
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<tr>
<td>10.40 - 11.20 AM</td>
<td>Prof. Ashutosh Sharma, IIT Kanpur and Secretary, DST, Govt of India</td>
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<td></td>
<td><em>Harnessing Self-organization in Confined Soft Materials for</em></td>
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<td></td>
<td><em>Micro/Nanofabrication</em></td>
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<tr>
<td>11.20 - 12.00 noon</td>
<td>Prof. Richard Friend, Cavendish Laboratory UK</td>
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<td></td>
<td><em>Excitons and charges in molecular semiconductors</em></td>
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<td>12.00 - 12.40 PM</td>
<td>Prof. T.V. Ramakrishnan, BHU Varanasi</td>
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<td></td>
<td><em>Learning About Quantum Spin Liquids</em></td>
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<tr>
<td>12.40 - 2.00 PM</td>
<td>Lunch at Main Guest House Reception Area, IISc Campus</td>
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<tr>
<td>2.00 - 2.40 PM</td>
<td>Technical Session: II (Chaired by Prof. S. Asokan)</td>
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<tr>
<td>2.00 - 2.40 PM</td>
<td>Prof. Eric Freysz, LOMA France</td>
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<td><em>THz nonlinear optics in condensed matter</em></td>
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<td>2.40 - 3.20 PM</td>
<td>Prof. D.D. Sarma, IISc Bangalore</td>
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<td><em>Electronic structure of the elusive metastable state in chemically</em></td>
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<td><em>exfoliated few layer MoS$_2$</em></td>
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<td>3.20 - 4.00 PM</td>
<td>Prof. Sriram Ramaswamy, TCIS TIFR Hyderabad and IISc Bangalore</td>
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<td><em>Flocks with inertia: asymmetric exchange and information transfer</em></td>
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<td>4.00 - 4.30 PM</td>
<td>Tea / Coffee break</td>
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<tr>
<td>4.30 - 5.30 PM</td>
<td>Felicitation program for Prof. A.K. Sood</td>
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<td>7.00 PM onwards</td>
<td>Conference Dinner</td>
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<td>Session</td>
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<td>9.10 - 9.50 AM</td>
<td>Technical Session: III (Chaired by Prof. Surajit Sengupta)</td>
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<td>10.30 - 11.10 AM</td>
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<td>11.10 - 11.30 AM</td>
<td>Tea / Coffee break</td>
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<tr>
<td>11.30 - 12.10 PM</td>
<td>Technical Session: IV (Chaired by Prof. S. Umapathy)</td>
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<tr>
<td>1.30 - 2.30 PM</td>
<td>Lunch Break</td>
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<tr>
<td>2.30 - 3.10 PM</td>
<td>Technical Session: V (Chaired by Prof. S.V. Bhat)</td>
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<td>5.10 - 5.30 PM</td>
<td>Tea / Coffee break</td>
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<td>5.30 - 6.15 PM</td>
<td>Evening lecture by Prof. Arun Grover, Panjab University</td>
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<td>7.30 PM onwards</td>
<td>Banquet</td>
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June 15th Wednesday (Venue: Physics Dept Auditorium, IISc)

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<thead>
<tr>
<th>Time</th>
<th>Technical Session: VI (Chaired by Prof. V.A. Raghunathan)</th>
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| 9.10 - 9.50 AM | Prof. Prabal K Maiti, IISc Bangalore  
Structure, dynamics and thermodynamics of water under nano-confinement                                               |
| 9.50 - 10.30 AM | Prof. P.V. Satyam, IOP Bhubaneswar  
Anisotropy Driven Hetero-Nanostructures (SiGe and AuAg) on High Index Silicon Substrates                               |
| 10.30 - 11.10 AM | Prof. Rajesh Ganapathy, JNCASR Bangalore  
Template-directed Self-Assembly of Colloidal Crystals                                                                           |
| 11.10 - 11.30 AM | **Tea / Coffee break**                                                                                                  |
| 11.30 - 12.10 PM | Technical Session: VII (Chaired by Prof. Anil Kumar)  
Prediction of robust non-centrosymmetric topological Dirac semi-metallic state in ternary half-Heusler compounds       |
| 12.10 - 12.50 PM | Prof. Surjeet Singh, IISER Pune  
The Pyrochlore Oxides: from geometrical frustration to interesting topological properties                              |
| 12.50 - 1.30 PM | Prof. Rema Krishnaswamy, Azim Premji University, Bangalore  
Yielding and structural transitions in sheared soft matter                                                                     |
| 1.30 - 2.30 PM  | **Concluding session followed by Lunch**                                                                                 |
Harnessing Self-organization in Confined Soft Materials for Micro/Nanofabrication

Ashutosh Sharma
Department of Chemical Engineering, Indian Institute of Technology, Kanpur;
Department of Science and Technology, Government of India

Micro/nano fabrication across a variety of materials and length scales remains a challenge which impacts important advances in functional interfaces, energy, electronics, health and environment. This talk will summarize some of our recent work on: (a) glassy carbon based structures and (b) understanding and control of self-organization, structure formation and instabilities in highly confined soft materials such as thin films and fibers. Applications range from functional coatings, cell-scaffolds, biosensors, actives delivery, energy storage, nanolens and nanowire arrays to a reusable pressure sensitive adhesive.

Selected Recent Publications:


Excitons and charges in molecular semiconductors

Richard Friend
Cavendish Laboratory
University of Cambridge

The physics of organic semiconductors is often controlled by large electron-hole Coulomb interactions and by large spin exchange energies. Photogenerated excitations are generally found to be strongly bound excitons, so that operation of an organic photovoltaic diode requires a donor-acceptor heterojunction that can split a photogenerated exciton to an electron-hole pair. In order to achieve long range charge separation, it is necessary to move these charges beyond the range of the Coulomb interaction between electron and hole, a distance of 5 nm or more. We have found that it is possible to measure the Coulomb energy set up as the electron-hole pair separate, through the modulation of the ground-state optical absorption of the donor caused by the local electric field set up between the electron and hole for a range of systems that use fullerenes as the electron acceptor. We found a substantial electron-hole separation at very early times, setting up an electrostatic field energy of up to 200 meV in times as short as 40 fsecs. We consider that this arises through direct electron transfer from donor to acceptor states that are delocalised over many acceptor molecules, over distances of 4 nm or more. I will report recent work that reveals this process to be general for a range of systems including those with non-fullerene acceptors. I will report also some recent observations of the process of ionisation of triplet excitons (generated via fission of triplet pairs from photogenerated singlet excitons) at all-organic donor acceptor heterojunctions formed with pentacene, based on structures we have previously reported. An alternative approach is to transfer the triplet exciton itself to a luminescent material and we have explored transfer of triplet excitons from pentacene to lead selenide nanocrystals.

Learning About Quantum Spin Liquids

T V Ramakrishnan
Department of Physics, Indian Institute of Science, Bangalore
Department of Physics, Banaras Hindu University, Varanasi

One of the things I learned from Ajay Sood is that quantum spin liquids actually exist. He measured the Raman spectra of two of them, both iridates, and found that they are unusually broad and smooth. The first, Na$_{1-x}$Li$_x$Ir$_2$O$_7$, can be thought of having a two dimensional honeycomb lattice for our purposes. While it is structurally and chemically a natural candidate for Kitaev like spin interactions, the identification is not automatic because the ground state is not a spin liquid, but a kind of spin solid, with magnetic long range order. A mean field theory for a Kitaev-Heisenberg spin system used to calculate the Raman response shows the persistence of Kitaev like correlations, and is in agreement with experiment. Another case is of Na$_4$Ir$_3$O$_8$ which has a 3d hyperkagome lattice structure and does not seem to have magnetic long range order. Again, a mixed Kitaev-Heisenberg model calculation of the Raman response reproduces not only the broad spectrum features and the shape, but also the peaks.

2. S.N.Gupta, P.V.Sriluckshmy, A.Balodhi, S.R.Hassan, Y.Singh, T.V.Ramakrishnan and AK Sood (to be submitted)
THz nonlinear optics in condensed matter
E. Freysz¹²

¹ Univ. de Bordeaux, LOMA, UMR 5798, 351 cours de la Libération, 33405 Talence Cedex, France
² CNRS, LOMA, UMR 5798, 351 cours de la Libération, 33405 Talence Cedex, France

In this seminar, we will present different experiments showing that THz nonlinear optics can be easily be performed in condensed phase matter. The THz frequencies belong to Far-Infrared radiations. They make it possible to characterize specifically far-infrared absorption bands occurring in condensed matters. While nowadays, linear THz spectroscopy is well developed; non linear THz optics and spectroscopy are still in progress mainly due to the lack to powerful THz sources. In this presentation, we will give an overview of the different powerful THz sources in use in our laboratory. Then we will demonstrate they can be used to performed original second-order and third-order nonlinear optical experiments in cubic nonlinear crystals belonging to 3m point group namely GaP and ZnTe. Using these crystals, we will demonstrate single-cycle THz pulses make it possible to fully characterize ultra-short femtosecond pulses [1], observe THz Kerr effect [2,3] or to induce second harmonic generation [4]. Finally, some of the prospects we have around time-resolved spectroscopy in condensed matter will be discussed.

Electronic structure of the elusive metastable state in chemically exfoliated few layer MoS$_2$

D. D. Sarma  
Solid State and Structural Chemistry Unit  
Indian Institute of Science, Bengaluru 560012

An elusive metastable phase, existing only as small patches in chemically exfoliated few layer, thermodynamically stable 2H phase of MoS$_2$ is believed to influence critically properties of MoS$_2$ based devices. Its electronic structure is little understood in absence of any direct experimental data and conflicting claims from theoretical investigations. I shall present data to resolve this issue based on probing the electronic structure of chemically exfoliated few layer systems using spatially resolved photoemission spectroscopy.

Flocks with inertia: asymmetric exchange and information transfer

Sriram Ramaswamy  
TCIS TIFR-Hyderabad

I will discuss the possible role of rotational inertia in models of spontaneously aligning groups of self-propelled particles. Excitations resembling second sound, sound propagation gaps, and instabilities arising from the analogue of a non-symmetric exchange interaction are among the results I will discuss.

Towards large-area synthesis of 2D materials

Young Hee Lee*  
Center for Integrated Nanostructure Physics, Institute for Basic Science, Sungkyunkwan University, Suwon, 440-746, Korea

In addition to metallic graphene monolayer, insulating hexagonal-BN monolayer and semiconducting layered transition metal dichalcogenides (LTMDs) are new classes of transparent and flexible materials, which can be used as essential components of transistors for soft electronics. While large-area graphene is available in a meter-scale, synthesis of large area monolayer h-BN and LTMDs are still a long way to realize. These materials have known to exhibit exotic physical and chemical phenomena which have never been accessed so far with 3D materials. We will discuss wafer-scale singlecrystalline monolayer graphene synthesis on Cu(111) substrate using tradition chemical vapour deposition and extend this idea to get AB-stacking bilayer graphene. Synthesis of BN requires different substrate, for example Pt, Au and Fe. We will also demonstrate a universal method of LTMDs of MX$_2$ (M=Mo, W, X=S, Se) using an idea of promoter with liquid precursor as a source. This allows uniform LTMDs in a wafer scale. If time is allowed, general synthesis approach of MoTe$_2$ will be also described.

*E-mail: leeyoung@skku.edu
Self-Assembly of Nanoparticle Superlattices and Membranes

Jin Wang
Argonne National Laboratory

Critical photonic, electronic, and magnetic applications of two-dimensional nanocrystal superlattices often require nanostructures in perfect single-crystal phases with long-range order and limited defects. Self-assembly of nanoparticles at fluid interfaces has emerged as a simple yet efficient way to create two-dimensional (2D) superlattices with tunable properties. Although the microscopic mechanism for self-organization of ligand-stabilized nanocrystals has been well established, the macroscopic patterns created by such interactions vary dramatically under different conditions. Even for a simple case of evaporating a colloidal droplet of nanocrystals on a surface, a variety of patterns has been reported, ranging from ordered 2D, three-dimensional (3D) nanocrystal superlattices, and fractal-like aggregates to percolated networks. Having such vastly different structures of nanocrystal assembly hinders the exploration of their physical properties, as well as creating obstacles for device applications. It is therefore essential to further understand and control the nanocrystal self-assembly mechanism. By using \textit{in situ} time-resolved x-ray scattering, we now can visualize the nucleation and growth kinetics of highly ordered nanocrystal superlattices at the interface of nanocrystal colloidal droplets. We discovered a crystalline phase with quasi-long-range positional order for two-dimensional nanocrystal superlattice domains self-assembled at the liquid-air interface during droplet evaporation. Recently, we showed that nanoparticle membranes formed at air/water interfaces exhibit a small (sub-nm) but significant difference in average ligand-shell thickness between their two sides. Molecular dynamics simulations elucidate the roles of ligand coverage and mobility in producing and maintaining this asymmetry. Understanding this Janus-like membrane asymmetry opens up new avenues for designing nanoparticle superstructures.

A successful collaboration on studying dynamics of nanoparticles with Professor Sood almost 20 years ago led me into the world of nanoparticles. To understand nanoparticle self-assembly and dynamics has become one of my research interests. The work described here has been a result of collaboration with my fellow Argonne scientists Dr. Xiao-min Lin, Zhang Jiang, Suresh Narayanan, et al. The work and the use of the Advanced Photon Source at Argonne National Laboratory were supported by US Department of Energy, Office of Science, Office of Basic Energy Sciences User Facility under Contract No. DE-AC02-06CH11357.

Development of Quantum Metrology in India: a Few Baby Steps

R C Budhani
Department of Physics
Indian Institute of Technology Kanpur

The standards of measurements are as old as the human civilization itself as they have evolved with time in the footsteps of the human race. Over the past half century, a mature understanding of the quantum properties of matter and the development of techniques to manipulate such properties have naturally led to the concept of Quantum Standards of measurements. Unlike the artifact based standards, the Quantum Standards are expected to remain invariant under space – time alterations. In this talk we will present the strategy that was adopted for the development of quantum standards of measurements for the seven base units of Standard Internationale (SI) in India and some key achievements of the past six years with a focus on Time and quantum Electrical Metrology.
Quantum Fluctuation Theorem for dissipative Cyclotron Motion*

Sushanta Dattagupta

The fluctuation theorems which traditionally have been studied for classical systems have also received substantive attention in the quantum domain over the last decade or so. We report further progress by an explicit analysis of quantum features especially at low temperatures. The example chosen is that of a problem which has proven to be of great interest in the context of Landau diamagnetism, viz., the quantized motion of an electron in a magnetic field and in a dissipative environment. It is established from first principles that a carefully defined work operator $W$ has a Gaussian distribution even though the system has a four-dimensional phase space. The parameter $a$ in the fluctuation theorem: $p(W)/p(-W) = \exp (aW)$, depends on the system dynamics and has characteristic quantum features especially at low temperatures. Certain unique quantum attributes are also discussed.

* Based on work done with Girish S. Agarwal

Nanostructures, Femtoseconds and Terawatts

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grk@tifr.res.in

High intensity, ultrashort light pulses are revolutionizing science and technology in very exciting ways, whether it is laboratory simulation of astrophysical phenomena, relativistic optics, particle acceleration on a table top, real time x-ray diffraction of the condensed phase or medical therapies for cancer. Such pulses can heat a piece of matter to intra-stellar temperatures at high density. It is this feature of ultrashort pulses that helps us study the behaviour of matter pushed to extreme conditions, in the laboratory.

Quite interestingly, the nano spatial scale has a very important role play in the interaction of intense, pulsed light with matter. We will present a variety of examples of how nanoparticles, nanowires and nanotubes influence MeV electron, megampere current pulse generation and its transport though dense, hot matter. We will illustrate the importance of the high ‘intensity contrast’ of the laser pulse in preserving the integrity of the nanostructures. We will provide pointers to the next generation of compact, bright, high energy charged particle and electromagnetic radiation sources and how they might change the way we do science and technology.

References:
    Also in Pramana- Journal of Physics, 73, p 113-155 (2009)  [Review]
[6] G. Chatterjee et al., (Submitted)
Molecular motor traffic: collective macro-molecular non-equilibrium phenomena in living matter

Debashish Chowdhury

Physics Department,
IIT, Kanpur

Specialized molecular motors called ribosome move forward along a mRNA track, utilizing input chemical energy, while synthesizing a protein using the track as a template. These movements are synchronized with the collective transit of a class of adapter molecules called tRNA through the space between two dynamic subunits of the ribosome. At a higher level the ribosomes themselves exhibit a traffic-like phenomenon while moving collectively on a given mRNA track synthesizing distinct copies of identical proteins. At the next higher level ribosome motors involved in the synthesis of different proteins interfere thereby regulating synthesis of those proteins. In this talk I'll present results obtained from theoretical models of some of these phenomena that we have developed in recent years. Our works, which extend the principles of non-equilibrium statistical physics of interacting self-propelled rods, provide insight into the spatio-temporal organization of the ribosomes and their activities in a living cell, the smallest unit of living matter.

Magneto-transport in the Topological Insulator Bi$_2$Se$_3$: Role of defects and disorder

C.S. Sundar

Materials Science Group,
Indira Gandhi Centre for Atomic Research, Kalpakkam 603 102

While the pioneering experiments on topological insulators using angle resolved photoemission spectroscopy has provided an unambiguous evidence for the presence of Dirac dispersed 2D states, the current interest in this field has shifted to exploring the novel transport properties of the topological surface states (TSS). The signatures of the topological surface state in transport experiments is often masked by the presence of a parallel bulk conductance path (due to defects such as anti-site disorder and vacancies), and the formation of two dimensional electron gas states at the bulk/surface interface due to band bending. Consequently, a major research effort has focused on the shifting the Fermi level into the bulk band-gap and thereby accessing the TSS in transport measurements.

In the present talk, we present the results of magneto-transport measurements in the topological insulating system, Bi$_2$Se$_3$, to explore the role of defects and disorder. Experiments have been carried out on single crystals synthesized under different conditions by varying the Se/Bi stoichiometry, cooling from melt at different rates, to control the Se vacancy concentration, and on the Sb and Te doped systems. Magneto-transport measurements have been carried out on single crystals in the temperature range of 4.2 K to 300 K and 0 T to 15 T magnetic field range, coupled with characterization of structure and defects using XRD and positron annihilation spectroscopy.

It is shown that the presence of defects influences the observation of Shubnikov-de Hass oscillation (SdH) oscillations characteristic of the topological surface state. Further, in the case of Te doping, the SdH oscillations gets suppressed and the magneto-resistance shows a cusp like positive magneto-resistance at
low magnetic fields and low temperatures, a feature associated with weak anti-localisation (WAL), that crosses over to negative magneto-resistance at higher fields. The qualitatively different magneto-transport behaviour seen in Bi$_2$SeTe$_2$ as compared to Bi$_2$Se$_3$ is rationalised in terms of the disorder, through an estimate of the carrier density, carrier mobility from Hall Effect measurements and an analysis in terms of the Ioffe-Regel criterion.

@Work done in collaboration with T R Devidas, E P Amaladass, Shilpam Sharma, Awadhesh Mani and A. Bharathi.

Jamming - unjamming transition and fluctuation relations associated with the driven vortex matter in 2H-NbS2 single crystals

Satyajit Banerjee
Department of Physics IIT Kanpur

Our recent measurement on velocity fluctuations in the driven vortex state in 2H-NbS2 (Tc = 6 K) single crystals have revealed signatures of random organization in the driven vortex state. Electrical transport measurements and evolution of velocity fluctuations in time series measurements, illustrate how flow in the driven vortex state naturally organizes into an immobile, zero velocity (jammed) state, by either waiting for long enough time and/or effectively applying a large drive. The dynamically generated zero-velocity state has properties distinct from the pristine pinned vortex state. Attempts to depin (unjam) this immobile vortex state into a uniform vortex flow regime have revealed (i) a novel moving phase fluctuating between a flowing and immobile state and (ii) diverging time scales and a critical like behaviour in the transient time scale vs driving force near the unjamming threshold force. The nature of the critical like behavior in a non equilibrium driven system indicates that the dynamical transition in the driven vortex state has features shared with other systems within the same universality class of driven non-equilibrium systems. The vortex-velocity distributions of driven vortex matter vividly demonstrate an underlying bimodal characeter, a useful basis for chaotic motion in the plastic flow regime. The immobile state of the vortex matter is akin to a Jammed vortex state. Apart from the above features the unjamming transition is also unusual. Here we identify events associated with the moving vortices corresponding to power consuming as well as unusual power generating events. Recently we have analysed these fluctuations associated with the non-equilibrium Jamming transition using the Gallavotti- Cohen fluctuation relations. We also show regimes where the fluctuation relation fails. We identify for the the first time the nature of the large deviation function associated with a non - equilibrium jamming transition in the driven vortex matter and also determine an effective non - equilibrium temperature scale associated with the unjamming transition. Through these studies the vortex matter emerges as a novel prototypical system for investigating features associated with non-equilibrium phase transitions. The work is a culmination of a long collaboration between my lab at IIT Kanpur, Prof. Arun K Grovers lab in TIFR and Prof. Ajay K. Sood's lab at IISc.
Science and applications of van der Waals materials assembly

Rahul R. Nair
School of Physics and Astronomy, University of Manchester, Manchester, UK

Van der Waals assembly of two-dimensional crystals continue attract intense interest due to the prospect of designing novel materials with on-demand properties. In my talk, I will mainly discuss various scientific and technological applications of van der Waals materials assembly. For example, the topic includes van der Waals pressure and its effects on trapped interlayer molecules at the 2D interface, superconductivity in graphene based laminate and applications of graphene based laminates for molecular separations.

References
1. K. S. Vasu et al., arXiv:1605.07106
3. Nair et al., Science 335, 442,(2012)

Long-range Attraction between Like-charged Colloids: Simulations and Microgravity Experiments

B. V. R. Tata
Condensed Matter Physics Division, Indira Gandhi Centre for Atomic Research, Kalpakkam 603102, Tamil Nadu
tata@igcar.gov.in

Deionized dilute charged colloidal systems exhibit gas-liquid, gas-solid and re-entrant transitions depending on suspensions parameters such as volume fraction, charge density and ionic strength. Occurrence of these transitions suggest the existence of long-range attraction between like-charged colloids and Monte Carlo (MC) simulations using a pair-potential, $U_s(r)$ having an attractive term in addition to the usual screened Coulomb term, could explain their occurrence. Observation of stable bound pairs in highly charged dilute polystyrene colloids with monovalent $H^+$ ions as counterions has provided direct evidence for the existence of long-range attractive term in $U(r)$ of like-charged colloids. Despite these reports, colloidal community is in search of additional evidences for existence of attraction between like-charged colloids which are free from sedimentation due to gravity and tethering. MC simulations on deionized charged colloids have revealed coexistence of liquid-like droplets with rare phase (gas-like) and voids coexisting with dense (solid-like) phase clusters, under zero gravity conditions. Ongoing “Kikuchi-Kossel” colloidal project funded by Japan Aerospace exploration Agency (JAXA), aims at verifying some of the above mentioned predictions by investigating the phase behavior of inorganic charged colloidal systems of different charge densities under microgravity conditions at International Space Station (ISS)/KIBO.
HARBINGERS OF HIGHER EDUCATION & RESEARCH AND NATIONAL DEVELOPMENT IN INDEPENDENT INDIA : A SELECTIVE COMPREHENSION

Arun K Grover*

Panjab University, Chandigarh -160014

P S Narayanan Memorial Lecture

I shall share a description connecting the following dots: (i) Addition of Punjab to British administered territories (1849), (ii) commencement of monitoring of education in schools in all regions under colonial rule (1854), (iii) initiation of affiliating Universities in Calcutta, Madras and Bombay (1857), (iv) University Acts (1860 & 1904), (v) establishing Government Colleges in Lahore and Delhi (1864), (vi) permitting creation of a constituent college of Calcutta University at Lahore and establishing Central College at Allahabad (1869), which progressed to become University of Panjab at Lahore in 1882 and University of Allahabad in 1887, respectively, (vii) encouraging College teachers to take study leave abroad, inviting faculty from England to visit Indian institutions and permitting appointment of Professors in Universities (1904), (viii) establishment of BHU (1916), University of Mysore (1916), Osmania (1918) and AMU (1920), (ix) Dr. Shanti Swarup Bhatnagar (SSB) as Research Professor at BHU (1921-24) and as founder Director University Chemical Laboratories, Lahore (1925-39), (x) creation of CSIR by SSB (1942), (xi) initiation of TIFR by Dr. Homi Bhabha at IISc campus (June 1, 1945) and its formal inauguration at Bombay (19.12.1945), (xii) formation of Committee for Atomic research in CSIR (1945), (xiii) creation of Atomic Energy Commission (1948), (xiii) synergy between Bhatnagar & Bhabha, (xiv) creation of UGC with SSB as its first Chairperson (1953), (xv) establishment of ISI by P C Mahalanobis (PCM) & his colleagues (1932) and his contributions of PCM to Five year Plans in independent India (1955-67), and (xvi) contributions of the architect of Green revolution, Dr B P Pal, to IARI, and the human resource development in agricultural sciences. Bhatnagar (1894-1955), Bhabha (1909-1966), Mahalanobis (1893-1973) and BP Pal (1906-1989) were four titans, all elected as FRS, and had much in common as personal characteristics.

*On leave of absence from Tata Institute of Fundamental Research (TIFR), Mumbai

Structure, dynamics and thermodynamics of water under nano-confinement

Prabal K Maiti

Center for Condensed Matter Theory, Department of Physics,
Indian Institute of Science, Bangalore, India.

We study the various translational and orientational dynamics of water molecules confined inside carbon nanotube using atomistic Molecular dynamics simulation (MD). The water molecules inside the nanotube show solid-like ordering at room temperature and surprisingly exhibit Fickian diffusion instead of single-file even if the particles can not cross one another. We propose model systems where single-file diffusion can be observed and test the prediction doing simulation in a nanoring. The confinement leads to strong anisotropy in the reorientational relaxation of the confined water molecules. The time scale of the relaxation of the dipolar correlations become ultra-slow. In contrast, the relaxation of the vector that joins the two hydrogens in a molecule becomes much faster. We also give the thermodynamics of water entry inside hydrophobic nanotube by calculating the Helmholtz free energy of water using two-phase thermodynamic (2PT) method.
Anisotropy Driven Hetero-Nanostructures (SiGe and AuAg) on High Index Silicon Substrates


In this talk, the shape evolution of MBE grown Si$_{1-x}$Ge$_x$ islands on ultraclean reconstructed high index Si(5 5 12) surfaces has been studied experimentally and explained using a phenomenological kinetic Monte Carlo (kMC) simulation. We show that a self-assembled growth at optimum thickness leads to interesting shape transformations, namely spherical islands to rectangular rods up to a critical size beyond which the symmetry of the structures is broken, resulting in a shape transition to elongated trapezoidal structures.

Similarly, a simple method to manipulate the bimetallic nanostructures (AuAg on Silicon) composition, size and shape using reconstructed high index (vicinal) surface as templates and ultrathin layers of noble metals (Ag) as seed atoms. The shape evaluation of MBE grown AuAg islands on ultra-clean reconstructed high index Si(5 5 12) surfaces with a variable thickness (0 to 1.25 ML) of Ag as seed layer has been studied experimentally and explained using a phenomenological kinetic Monte Carlo (kMC) simulation. An order of magnitude higher aspect ratio for AuAg nanowires is observed with presence of about 1.2 ML of Ag as seed layer on Si (5 5 12). Both the MBE experiments and kMC simulations suggest an increase of aspect ratio up to a thickness of $\sim$0.8 ML Ag seed layer and there after the average aspect ratio saturates. Anisotropic diffusion across the steps and terraces and enhanced mobility of Ag compared to Au, lead to the formation of high aspect ratio AuAg nanowires.

Template-directed Self-Assembly of Colloidal Crystals

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Site-specific colloidal crystal nucleation and subsequent control over the size and symmetry of the growing crystallites is of considerable importance for a wide variety of applications that include structural color, optoelectronics, and composites. While for atomic and molecular systems, heteroepitaxy and/or epitaxy over patterned substrates allows exquisite control over most of the above parameters, for micrometer-sized colloidal particles, owing to their slow dynamics, attempts to achieve control over these parameters continues to remain challenging. In this talk, I will describe recent results wherein we design templates with binding energy gradients to achieve site-specific crystal nucleation. Colloidal particles on these surfaces migrate to specific-sites prior to subsequent nucleation and subsequent growth. I will also highlight similarities and difference between colloids and atomic systems.
Prediction of robust non-centrosymmetric topological Dirac semi-metallic state in ternary half-Heusler compounds

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Theoretical analysis of topological character of the quantum structure of electrons in a crystal and prediction of their exotic transport, magnetic, chiral and superconducting properties have led to profuse research in the last decade, and discovery of topological insulators, Weyl and Dirac semi-metals. A Topological Dirac semi-metal (TDSM), a 3-dimensional analogue of graphene, is particularly interesting as a parent to other topological states. While many materials have been predicted to be topological Dirac Semi-metals, they are often centro-symmetric and not easy to make. Here, we present a generic topological phase diagram of a large family of half-Heusler compounds with strained structures maintaining a three-fold symmetry, and discover their highly robust non-centrosymmetric TDSM state. Using an existing half-Heusler LiMgBi as a model system in first-principles theoretical analysis, we show that isotropic compression stabilizes a normal insulating state with ionic character, while axial compression along a three-fold symmetry axis stabilizes the TDSM state. Secondly, symmetry of its valence and conduction bands permits a gap-preserving transition with axial tension from its normal to topological insulating state. Showing how insulators can arise from only metallic constituents and uncovering many half-Heuslers exhibiting Dirac semi-metallic and other topological states, our work opens up tremendous possibilities of their epitaxial hetero-structures and interfaces that involve chirality, polarity, topology and correlations.

Keywords: Electronic Topology, Phase Transition, Topological Dirac Semi-metal, Topological Insulator, Novel metals.

The Pyrochlore Oxides: from geometrical frustration to interesting topological properties

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The Pyrochlore oxides are well-known to show complex magnetic ground states due to geometrical frustration arising from their corner-linked tetrahedral structure. One of these states which attracted considerable attention recently is called the spin ice; because its spin structure can be mapped onto the proton positions in the water ice. In this talk, I will discuss our experimental results on the spin ice compound Dy2Ti2O7 (DTO). More specifically, using a combination of low-temperature Raman and XRD, we showed that DTO exhibits a subtle structural distortion around 100 K. However, the distortion seems not to have any obvious bearing on the spin ice physics. The second system that I will discuss is a metallic pyrochlore Sm2Mo2O7 (SMO), which we propose to be a metallic spin ice. And, finally, I will show some results from our ongoing work (mainly structural characteristics) on the potential Weyl semi-metal Eu2Ir2O7 (EIO). In our experiments, we discovered a very unusual volume collapse of the EIO lattice upon Bi-doping (2-3 at. %), with no evidence for any structural change.
Yielding and structural transitions in sheared soft matter

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The rich non-linear flow behaviour of Soft Matter systems under shear is closely linked to the structure and dynamics at mesoscopic length scales. I will present a microscopic view of two distinct shear induced effects in soft matter: i) an elastic to plastic flow (yielding) under periodic shear and ii) nonequilibrium phase transitions under steady shear accompanied by flow instabilities.

The first part of the talk will discuss the macroscopic yielding behaviour of a non-particulate amorphous solid formed by a Langmuir monolayer of an insoluble surfactant, subjected to a periodic shear over a large number of shear cycles. The transient dynamics reveal signatures of a nonequilibrium transition well above the onset of nonlinearity (yield point) in the stress-strain rheological curve. I will present a microscopic view of the yielding obtained through particle imaging velocimetry techniques, which suggests that the critical-like behaviour of the macroscopic rheological parameters arises from the change in the flow field within the monolayer from a linear shear flow to a power law flow behaviour at the onset of fluidization.

The second part of the talk will discuss the structural transitions in a lyotropic lamellar phase and emphasize the role of synchrotron X-ray scattering studies in following the kinetics of the transition. I will show how the coupling of shear with membrane curvature defects in bilayers can lead to ordering, melting or hydrodynamic instabilities in the surfactant mesophase.