Annual Report 2012-13

TIFR Centre for Interdisciplinary Sciences

V. Chandrasekhar

Highlights

Molecular Materials

- We have been involved in the of molecular systems that can show molecular magnetism.
- We have designed strategies for preparing complex molecular entities containing homo-(3d and 4f) and heterometallic (3d-4f) systems (Figure 1).
- Some of these compounds have been shown to possess single-molecule magnet properties.

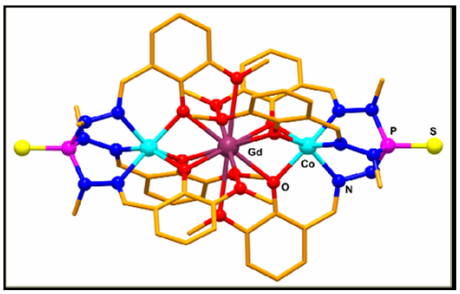

Figure 1: A heterometallic trinuclear Co2Gd complex

We have worked on cyclometalated Ir(III) compounds with particular emphasis on hetero-bridged dinuclear derivatives with a view to improve their photophysical properties. In these systems we were able to prepare a family of compounds whose emission properties could be modulated from green to red.

Molecular and Supramolecular Chemistry

Utilizing multi-topic ligands such as organophosphonates and organophosphates we have been able to assemble exotic molecular aggregates, The nuclearity of the molecular systems can be varied by a changing the steric bulk of the ligands as well as introducing ancillary nitrogen ligands (Figure 2).

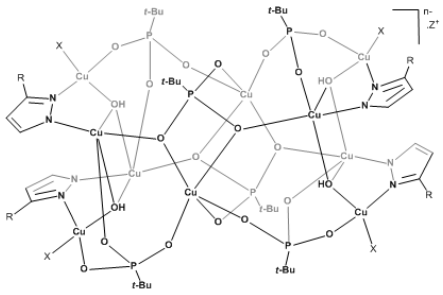

Figure 2: A decanuclear Cu(II) phosphonate containing pyrazole ligands.

Invited Talks in Conferences and Meetings

- Molecules to Materials: A Synthetic Chemist's Perspective TCIS, Inaugural Symposium, August 6, 2012.
- Phosphorus-supported Ligands for the Assembly of Molecule-based Magnetic Materials The 13th International Conference on Molecule-based Magnets Orlando, USA, October 7- October 11 2012
- The Utility of Phosphorus-supported Ligands in Assembling Heterometallic 3d/4f Complexes Electronic, Optical and Magnetic Molecular Materials: Experiments and Modeling Orange County, Coorg, November 25-28 2012
- Phosphorus-supported Ligands for the Assembly of Molecule-based Magnetic Materials JNCASR Meeting on Chemistry of Materials Trivandrum, September 30- October 2 2012
- Phosphorus-supported Ligands for the Assembly of Molecule-based Magnetic Materials Complex Chemical Systems IISER Bhopal, December 3-5 2012
- Phosphorus-supported Ligands for the Assembly of Molecule-based Magnetic Materials New Directions in Complex Chemical Systems IIT Delhi, December 7-9 2012
- Phosphorus-supported Ligands for the Assembly of Molecule-based Magnetic Materials Chemistry: Synthesis, Structure and Dynamics Orange County, Coorg, Karnataka, December 11-14 2012
- Chemistry, the Central Science Vigyanotsav, University of Hyderabad, January 18, 2013

- Organometallic Cyclometalated Ir (III) compounds: Synthesis, Structure and Photoluminescence Organometallic Chemistry Conference, KIIT, Bhubaneshwar, February 5-7, 2012
- Heterometallic (3d/4f) and homometallic (4f) ensembles: new families of molecule-based magnets Functional Metal Organics-2013 Kolkata Feb 8-10, 2013
- Single-Molecule Magnets Amrita Vishwavidyapeetham, Coimbatore, March 22, 2013

Publications (2012)

- Cyclophosphazene and cyclocarbophosphazene-based ligands V. Chandrasekhar, A. Dey, S. Kundu **Ind., J. Chem.**, 2012, 51, 118-129
- Distorted Cubic Tetranuclear Vanadium(IV) Phosphonate Cages: Double-four-ring (D4R) containing transition metal ion cages V. Chandrasekhar, A. Dey, T. Senapati, E. C. Sanudo **Dalton Trans.** 2012, 799-803
- Ligand-Bridged Dinuclear Cyclometalated IrIII Complexes: From Metallamacrocycles to Discrete Dimers V.Chandrasekhar, T. Hajra, J. K. Bera, S.M. Wahidur Rahaman, N. Satumtira, O. Elbjeirami, and M. A. Omary **Inorg. Chem.** 2012, 51, 1319-29
- Cyclo- and Carbophosphazene-Supported Ligands for the Assembly of Heterometallic (Cu2+/Ca2+, Cu2+/Dy3+, Cu2+/Tb3+) Complexes: Synthesis, Structure, and Magnetism V. Chandrasekhar, T. Senapati, Atanu Dey, Sourav Das, Marguerite Kalisz and Rodolphe Clerac **Inorg. Chem.** 2012, 51, 2031-38
- Multicomponent Assembly of Anionic and Neutral Decanuclear Copper(II) Phosphonate Cages V. Chandrasekhar, L. Nagarajan, S. Hossain, K. Gopal, S. Ghosh, S. Verma **Inorg. Chem.** 2012, 51, 5605-16
- Synthesis of One- and Two-Dimensional Coordination Polymers Containing Organotin Macrocycles. Reactions of (n-Bu3Sn)2O with Pyridine Dicarboxylic Acids. Structure-Directing Role of the Ancillary 4,4 '-Bipyridine Ligand, V. Chandrasekhar, C. Mohapatra, R. J. Butcher **Crystal Growth and Design**, 2012, 12, 3285-95
- Carboxylate-free Manganese (II) Phosphonate Assemblies: Synthesis, Structure and Magnetism V. Chandrasekhar, J. Goura, E. C. Sanudo **Inorg. Chem.** 2012, 51, 8479-87
- Novel Chemosensor for the Visual Detection of Copper(II) in Aqueous Solution at the ppm Level V. Chandrasekhar, S. Das, R. Yadav, S.

Hossain, R. Parihar, G. Subramaniam, P. Sen **Inorg. Chem.** 2012, 51, 8664-66

- Bismuthferrocene carboxylates: Synthesis and Structure V. Chandrasekhar, R. K. Metre **Dalton. Trans.** 2012, 41, 1168411691

- Trapping Dimethyltin Cations by Bipyridine-N,N-Dioxide Ligands V. Chandrasekhar, P.Singh, K. Gopal, A. Steiner **Z. Anorg. Allg. Chem.** 2012, 638, 18

- Cyclometalated Iridium(III) Complexes Containing Hydroxide/Chloride Ligands: Isolation of Heterobridged Dinuclear Iridium(III) Compounds Containing -OH and -Pyrazole Ligands V. Chandrasekhar, B. Mahanti, P. Bandipalli, K. Bhanuprakash **Inorg. Chem.** 2012, 51, 10536-47.

Rama Govindarajan

Highlights

Fluid mechanics group:

- Vortex merger is an important mechanism for the inverse cascade of energy in turbulent flow. It was shown that merger can be delayed and even prevented by background density stratification.
- A drop of liquid moving down an inclined plate was shown to roll or slide in a ratio depending only on a shape factor and not on many other parameters.
- The film flowing down an inclined plate was shown to be very sensitive to Froude number Fr when Fr 1. In this regime, shallow water theory ws shown not to give the correct answers. (RG)

Staff List

1. Charudatt Kaushik: Project Assistant
2. Divya Venkataraman: Project Assistant
3. Shrikant Derebail: Project Assistant (under CEFIPRA)

National and International Involvement (Professional and Academic) Memberships of editorial, academic and national committees, Office bearership of professional societies, etc.

on the Editorial Board of Sadhana

- Member of a Panel of Experts, Science & Engineering Research Board (SERB), Department of Science & Technology (DST) Government of India.
- Member, Engineering Sciences Research Committee, Council for Scientific and Industrial Research (CSIR), Government of India.
- Member, Advisory Committee of the Chemical Engineering Department, IIT Hyderabad.
- Member, Indian National Committee for the Asian Congress of Fluid Mechanics, INCOAF.

Visits

To the Woods Hole Oceanographic Institution, as the 2012 Mary Sears Fellow. (Nov 2012).

Awards and Distinctions

Designated an Honorary Professor, Department of Mathematics, University of Hyderabad.

Non DAE Research Projects

Rama Govindarajan and Benoit Pier, Rotating and curved boundary layer instabilities. Indo-French Centre for the Promotion of Advanced Research (CEFIPRA) Jan 2013-Dec 2015.

Publications

- Stability of developing film flow down an inclined surface. Sarath Ramadurgam, RVK Chakravarthy, Gaurav Tomar & Rama Govindarajan, Physics of Fluids, **24**, 102109, (2012).
- Effect of density stratification on vortex merger. Harish Dixit & Rama Govindarajan, Physics of Fluids, **25**, 016601, (2013).
- Do liquid drops roll or slide on inclined surfaces? Sumesh P Thampi, R. Adhikari, and Rama Govindarajan, Langmuir, **29**, pp 33393346, (2013).

Lectures / Lecture Courses Given Elsewhere

- Introduction to Fluid Mechanics 3 lectures, DST-SERC (Department of Science and Technology Government of India, Science & Engineering Research Council) School on Nonlinear Dynamics, Kolkata December 2012.
- "Bridge mathematics" co-taught at the University of Hyderabad, August-December 2012.
- Seminars/ Colloquia at Harvard, Brown, UCSB, WHOI, University of Michigan.

Graduate Courses

Advanced Continuum Mechanics, co-taught.

Ph.D. Theses / M.Sc. Theses

- Singular Eigenfunctions in Hydrodynamic Stability: The Roles of Rotation, Stratification and Elasticity, Anubhab Roy. Co-advisor: Ganesh Subramanian. PhD JNCASR 2013.

- Drag reduction by surface-coating of cilia on airfoils. Divya Venkataraman. Co-advisor: Alessandro Bottaro, University of Genova.

Popular Science Articles / Lectures

"The Y in Phsics" Evening talks for undergraduate students at IIT Madras and in the Junior Science Club, University of Hyderabad.

Smarajit Karmakar

Highlights

Breakdown of the Stokes-Einstein relation in two, three and four dimensions

- The breakdown of the Stokes-Einstein (SE) relation between diffusivity and viscosity at low temperatures is considered to be one of the hallmarks of glassy dynamics in liquids. Theoretical analyses relate this breakdown with the presence of heterogeneous dynamics, and by extension, with the fragility of glass formers.

- We perform an investigation of the breakdown of the SE relation in 2,3 and 4 dimensions, in order to understand these interrelations. Results from simulations of model glass formers show that the degree of the breakdown of the SE relation decreases with increasing spatial dimensionality.

- The breakdown itself can be rationalized *via* the difference between the activation free energies for diffusivity and viscocity or relaxation times in the Adam-Gibbs relation.

- The fragility of the studied liquids is found to increase with spatial dimensionality, contrary to the expectation based on the association of fragility with heterogeneous dynamics.

- We calculate various measures of heterogeneity of dynamics and find no clear correlation between the degree of the SE breakdown and the heterogeneity of dynamics.

  Collaborators : Shiladitya Sengupta (JNCASR, Bangalore and TIFR-H, Hyderabad), **Smarajit Karmakar**, Chandan Dasgupta (IISc, Bangalore), Srikanth Sastry (JNCASR, Bangalore and TIFR-H, Hyderabad)

Random Pinning Glass Model

- Glass transition where viscosity of liquids increases dramatically upon decrease of temperature without any major change in structural properties, remains one of the most challenging problems in condensed matter physics in spite of tremendous research efforts in last decades.

- On the other hand disordered freezing of spins in a magnetic materials with decreasing temperature, the so-called spin glass transition, is relatively better understood. Previously found similarity between some spin glass models with the structural glasses inspired development of

theories of structural glasses based on the scenario of spin glass transition. This scenario though looks very appealing is still far from being well established.

- One of the main differences between standard spin systems to molecular systems is the absence of quenched disorder and the presence of translational invariance: it is often assumed that this difference is not relevant, but this conjecture still needs to be established.

- The quantities, which are well defined and characterized for spin models, are not easily calculable for molecular glasses due to the lack of quenched disorder which breaks the translational invariance in the system and the characterization of the similarity between the spin and the structural glass transition remained an elusive subject.

- In this study we introduced a model structural glass with built in quenched disorder which alleviates this main difference between the spin and molecular glasses thereby helping us to compare these two systems: the possibility of producing a good thermalization at rather low temperatures is one of the advantages of this model.

  Collaborators : Smarajit Karmakar (TIFR-H and Departimento di Fisica, Universitá di Roma "La Sapienza ",Roma, Italy) and Giorgio Parisi (Departimento di Fisica, Universitá di Roma "La Sapienza ",Roma, Italy)

Distribution of Diffusion Constants and Stokes-Einstein Violation in supercooled liquids

- It is widely believed that the breakdown of the Stokes-Einstein relation between the translational diffusivity and the shear viscosity in supercooled liquids is due to the development of dynamic heterogeneity *i.e.* the presence of both slow and fast moving particles in the system.

- In this study we *directly* calculate the distribution of the diffusivity for a model system for different temperatures in the supercooled regime. We find that with decreasing temperature, the distribution evolves from Gaussian to bimodal indicating that on the time scale of the α relaxation time, mobile (liquid like) and less mobile (solid like) particles in the system can be *unambiguously* identified. We also show that less mobile particles obey the Stokes-Einstein relation even in the supercooled regime and it is the mobile particles which show strong violation of the Stokes-Einstein relation.

- Finally, we show that the degree of violation of the Stokes-Einstein relation can be tuned by introducing randomly pinned particles in the system.

Collaborators : Shiladitya Sengupta (JNCASR, Bangalore and TIFR-H, Hyderabad) and **Smarajit Karmakar**

Identity of the length Scale Characterizing the Glass Transition from Different Approaches

- The dramatic dynamic slowing down associated with the glass transition indicates the existence of a static length scale that should grow rapidly when temperature decreases.
- It turned out that the definition and calculation of such a length scale is subtle and non-trivial. Recently there were two such definitions that seem to fit the bill, that were based on very different insights regarding the relevant physics. One approach is based on the point to set correlation technique and the other on the scale where the lowest eigenvalue of the Hessian matrix becomes sensitive to disorder.
- In this work we present evidence that the two approaches result in the same identical length scale. The two methods are complementary in being relevant for higher and lower temperature regimes respectively.

  Collaborators : Giulio Biroli (CEA Saclay, France), **Smarajit Karmakar** and Itamar Procaccia (Weizmann Institute of Sciences, Israel)

Publications

1. Breakdown of the Stokes-Einstein relation in two, three, and four dimensions - Shiladitya Sengupta, Smarajit Karmakar, Chandan Dasgupta, and Srikanth Sastry, J. Chem. Phys. **138**, 12A548 (2013).
2. Random Pinning Glass Model - Smarajit Karmakar and Giorgio Parisi, Proc. Nat. Acard. Sci (USA) www.pnas.org/cgi/doi/10.1073/pnas.1222848110. Smarajit Karmakar and Itamar Procaccia (manuscript to be submitted).

P.P. Rajeev

Highlights

Intense Laser Physics

The intense laser program for the TIFR Hyderabad campus is now initiated at TIFR Center for Interdisciplinary Sciences (TCIS). As part of this two Faculty members have joined TCIS. A 0.5 Terawatt laser lab is being setup now at TCIS, which will be used primarily for investigating behaviour of transparent matter under extreme conditions. We list the progress below:

Setting up a Terawatt Laser Laboratory

- Components for building a 0.5 Terawatt Laser were shipped earlier in the year from TIFR, Mumbai to the Hyderabad Campus. This laser is a custom-built system by Coherent and Continuum. As it is a fairly old system (more than 15 years old), it had to be reinstalled from scratch in TCIS.

- This has progressed quite successfully and we have achieved low energy, short pulses (5 nJ, 60fs) in the system in the reporting year. The plan for the next few months is to get these pulses amplified to the full spec of the laser.

- This laser system, once fully setup, will be used for several planned activities in TCIS such as:

  (a) Investigating attosecond dynamics inside solids
  (b) Probing nanoscale ionization and dynamics inside transparent materials and softmatter
  (c) XUV source development from clusters

(P. P. Rajeev, Ram Gopal and M. Krishnamurthy)

Figure 3: Dr. Ram Gopal aligning the femtosecond oscillator

Figure 4: The 0.5 TW laser system being assembled

Staff List

1. Dr. P. P. Rajeev and Prof. M. Krishnamurthy (Principal Investigators)
2. Dr. Ram Gopal (visiting Fellow)

National and International Involvement (Professional and Academic)

Dr. P. P. Rajeev has a collaboration with the Central Laser Facility, Rutherford Appleton Laboratory, UK, where he carries out cutting-edge experiments at extreme intensities

Graduate Courses

Experimental Methods course at TCIS

Popular Science Articles / Lectures

Light that matters: P. P. Rajeev at Mahavir Institute for Science and Technology, Hyderabad, 22nd March, 2013

Sriram Ramaswamy

Highlights

Active liquid crystals

Active matter refers to collections of interacting self-driven energy-dissipating particles. Obvious realizations include motor-filament complexes inside living cells, collections of organisms on all scales from microns to kilometers, and chemical or mechanical imitators of motility. Spatial organization in active systems is at the forefront of research in nonequilibrium and biological physics today. A particular case of interest is active striped phases, for which we constructed a hydrodynamic theory whose striking predictions included novel instabilities, enhanced order in 2 and 3 dimensions and reentrant Kosterlitz-Thouless melting to an active nematic in 2 dimensions (published in Phys Rev Letters, with T Adhyapak, PhD student, now postdoc at TU Berlin, and J Toner, Univ of Oregon).

The growth of glassy order

We extended the classic "mode-coupling" approach to the glass transition to the case of non-stationary states, allowing us to characterize the way glassiness grows. This is important both conceptually and as a further test of our theoretical understanding of the glass transition. Our predictions on the growth kinetics of a certain three-density correlator accounts remarkably well for old and hitherto not understood numerical observations (published in Phys Rev Letters, with S K Nandi, PhD student, now postdoc at Saclay).

Large deviations in yielding gels

We developed a simple statistical-mechanical theory of the strange phenomenon of negative strain rate fluctuations seen in experiments on surfactant gels, within which we find remarkable properties of the large-deviation function (LDF) for the velocity, including a non-quadratic form near yielding, and a steady-state fluctuation relation (FR) at small driving. Crucially, our approach suggests that large fluctuations and motion in a direction opposite to an imposed force are likely to occur in a wider class of systems near yielding (published in J Stat Mech: Theory and Applications, with S K Nandi, PhD student, B Chakraborty, Brandeis and A K Sood, IISc).

National and International Involvement (Professional and Academic) Memberships of editorial, academic and national committees, Office bearership of professional societies, etc.

Fellow of Indian Academy of Sciences since 1996, and Fellow of INSA since 2003.

Member, Editorial Boards of: *Annual Review of Condensed Matter Physics* since 2011, *Advances in Physics* since 2007, *European Physical Journal E* since 2009, *Journal of Statistical Mechanics: Theory and Experiment* since 2003; member, Advisory Board of *Soft Matter* since 2008.

Visits

Higgs Centre, University of Edinburgh, March 2013 (research collaboration with M E Cates and group)

Publications

a) In Journals:

- Yielding and large deviations in micellar gels: a model, S K Nandi, B Chakraborty, A K Sood and S Ramaswamy, J. Stat. Mech. (2013) P02027; `arXiv:1210.1987`
- Live Soap: Order, Fluctuations and Instabilities in Active Smectics, T.C. Adhyapak, S. Ramaswamy, and John Toner, `http://arxiv.org/abs/1204.2708`, Phys. Rev. Lett. **110** (2013) 118102
- Theory of the domain growth of glassy correlations, S.K. Nandi, S. Ramaswamy `http://arxiv.org/abs/1205.1152`, Phys Rev Lett, **109** (2012) 115702

Graduate Courses

- Statistical Mechanics of time dependent phenomena, Aug-Dec 2013
- Soft Condensed Matter, Jan-Apr 2013

Invited Talks in Conferences and Meetings

- Invited talk at "Mechanical manipulations and responses at the scale of the cell and beyond", NCBS, TIFR, Bangalore 19-21 April 2013.
- Invited talk at the conference "Self-organization and Emergent Dynamics in Active Soft Matter", Yukawa Institute for Theoretical Physics, Kyoto, 18-20 Feb 2013
- Invited talk at Conference on Condensed Matter and Biological Systems, BHU, Varanasi, 11-14 Jan 2013

- Invited talk at B12B, Silver Jubilee of CCMB, Hyderabad, 25-27 Nov 2012.
- Invited talk at workshop on Nonequilibrium collective dynamics – Bridging the gap between hard and soft materials, Potsdam, Germany, 1-4 Oct 2012.
- Invited talk at Workshop on Active Soft and Biological Matter, in honor of Jacques Prost, Les Houches, France, 30 Sep - 5 Oct 2012.
- Invited talk at Frontiers in Physics, University of Hyderabad, 27-28 Sep 2012
- Invited talk at De Gennes Days on Physics of Cells, from soft to living matter (PhysCell2012), Hyères, France, 4-7 Sep 2012

Popular Science Articles / Lectures

- Public Lecture at Science Day symposium, IISER Pune, 28 Feb 2013.
- Infosys Prize Public Lecture, University of Hyderabad, 25 Feb 2013.

Srikanth Sastry

Highlights

National and International Involvement (Professional and Academic) Memberships of editorial, academic and national committees, Office bearership of professional societies, etc.

Academic Committee, Raman Research Institute

Visits

Scientific visits to EPFL Lausanne, Switzerland, Monte Verita, Switzerland, WPI, Sendai, Japan, BHU, Banaras, Univ. Paris Sud Orsay, Uni. H. Heine, Dusseldorf, Germany, Univ. Erlangen, Germany, for scientific collaboration and conferences.

Invited Talks in Conferences and Meetings

- The AIMR Workshop Structure and Dynamics of Glass, WPI, Sendai, Japan, June 27 - 29, 2012.
- International Workshop on "Micro-structure, setting and aging of cement: from soft matter physics to sustainable materials.", Monte Verita, Switzerland, August 12 - 16, 2012.
- Conference On Condensed Matter and Biological Systems, BHU, Banaras, January 11-14, 2013.
- Erlangen workshop on 'Nonlinear response in Complex Matter', Erlangen, Germany, February 25-27, 2013.

Publications

(a) Shiladitya Sengupta, Smarajit Karmakar, Chandan Dasgupta and Srikanth Sastry, Adam-Gibbs Relation for Glass-Forming Liquids in Two, Three, and Four Dimensions, Phys. Rev. Lett. 109 095705 (2012).

(b) Vishwas V Vasisht and Srikanth Sastry, Liquid-Liquid Phase Transition in Supercooled Silicon, in "Liquid Polymorphism", Adv. Chem. Phys. vol. 152, p. 463 (2013).

(c) Francis W. Starr, Jack F. Douglas, Srikanth Sastry, The Relationship of Dynamical Heterogeneity to the Adam-Gibbs and Random First-Order Transition Theories of Glass Formation, J. Chem. Phys., 138, 12A541 (2013).

(d) Shiladitya Sengupta, Smarajit Karmakar, Chandan Dasgupta and Srikanth Sastry, Breakdown of the Stokes-Einstein Relation in Two, Three, and Four Dimensions, J. Chem. Phys. 138, 12A548 (2013).

(e) Moumita Maiti, Arun Laxminarayan and Srikanth Sastry, Characterization of Void Space in Polydisperse Sphere Packings: Applications to hard sphere packings and to protein structure analysis, E. Phys. J. E. 36: 5 (2013).

Graduate Courses

Computational Methods for Condensed Matter Systems: Aug - Dec 2012 Soft Mater: Equilibrium and Dynamics: Jan - April 2013

Ph.D. Theses / M.Sc. Theses

Moumita Maiti, Shiladitya Sengupta, Vishwas V Vasisht. JNCASR.

Surajit Sengupta

Highlights

Non-monotonic crossover from single-file to regular diffusion in micro-channels

It was found, both experimentally and in computer simulations that the dynamics of colloidal particles confined within a narrow channel depends in a complex fashion on the width of the channel. When the width is a commensurate multiple of the typical ordering length of the colloids, the particles diffuse in a single-file manner for a very long time, ultimately crossing over to regular diffusion. The crossover time decreases rapidly as the width is tuned away from commensuration. The experiments were performed in the group of P. Leiderer in the University of Konstanz in Germany and the computations involved collaboration between Surajit Sengupta of TCIS, Hyderabad and the group of P. Nielaba, Konstanz, Germany. The paper was published in Scientific Reports, an online journal of the Nature Publishing Group.

Dynamics of soft matter in micro channels:

The dynamics of plastically deformed solids, confined within micro-channels, was investigated using large scale computer simulations. Various regimes, including jamming, plug flow and plastic deformation was identified and the role of defects during this process was highlighted. In a separate investigation within the same theme, the diffusion of individual colloidal particles confined within micro-channels was investigated and was shown to have interesting cross-overs from single file to normal diffusion as a function of the width of the channel. These results were confirmed using laboratory experiments.

Thermodynamic anomalies in network formers:

Network forming materials like water, Si, silicate glasses as well as gels made out of patchy colloidal particles, show a number of thermodynamic anomalies like density maxima, pressure minima, anomalies in the compressibility etc. Many of these anomalies arise from local network structures formed in the liquid state. Many materials, chemical and biological processes depend on this network forming ability. In a set of computer simulations we investigated whether network formation may be influenced by manipulating external periodic fields or by the use of a template. Our results were understood in terms of a mean field calculation of a suitably constructed lattice model.

Staff List

Mr. Debabrata Sinha, graduate student

National and International Involvement (Professional and Academic) Memberships of editorial, academic and national committees, Office bearership of professional societies, etc.

Fellow of Indian Academy of Sciences and member of the Summer Research Fellowship Selection Committee.

Non DAE Research Projects

(a) Investigators: Chandan Dasgupta, IISc. Bangalore (PI), Surajit Sengupta, TCIS, Hyderabad (co PI), Oriol T Valls (co PI), U. Minnesota U.S.A. (co PI), John Toner U. Oregon, U.S.A.

(b) Title: Joint India-US Center on the Dynamics of Dislocations in Solid 4He and its Role in Supersolid Behavior

(c) Funding Agency: Indo-US Science and Technology Forum.

Duration: 3 years.

Publications

a) In Journals:

1. D. Wilms, P. Virnau, S. Sengupta and K. Binder, *Langevin dynamics simulations of a two-dimensional colloidal crystal under confinement and shear*, Phys. Rev. E **85**, 061406 (2012).

2. U.Siems, C.Kreuter, A.Erbe, N.Schwierz, S.Sengupta, P.Leiderer, P.Nielaba *Non-monotonic crossover from single-file to regular diffusion in micro-channels*, Scientific Reports (Nature Publishing Group) **2**, 1015 (2012).

3. Chandana Mondal and Surajit Sengupta *Thermodynamic anomalies of a network former in a periodic field.* Eur. Phys. J. E **36**, 6 (2013).

4. Jayee Bhattacharya, Vijay Singh, Surajit Sengupta and Indra Dasgupta *Magneto-structural transitions: Molecular dynamics simulations of a united-atom mesoscopic model*, Mod. Phys. Lett. B **27**, 1350047 (2013).

Conferences Organised by the Centre

- Chemistry Symposium, April 27, 2013.
- TCIS-IITH-IITB meeting on Flow Instability, January 3-4, 2013: an event bringing together groups at TCIS, and IIT Hyderabad, Madras and Bombay, working on nonlinear dynamics, instabilities and fluid flow.
- Meeting on Soft & Biological Matter, 28 Nov 2012, with several participants from the TIFR system and the Univ of Hyderabad
- TCIS Symposium, August 6 & 7, 2012, highlighting the range of activities in the Centre.

Lectures by Visitors

See TCIS web page http://www.tifrh.res.in/tcis/events/seminars.html