



SATYENDRA NATH BOSE NATIONAL CENTRE FOR BASIC SCIENCES

Newsletter



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Editorial

This issue brings in issues 2 and 3 together. Issue 2 could not be published earlier for a number of compelling reasons, like many of the editorial board members, mostly the student members, were busy in writing thesis and so on. Many of these members have already left which makes it mandatory to reconstitute the editorial board. The present issue reflects the academic environment prevailing in the institute through a large number of thesis presentations. The Bose Fest, different awards to the students add to the vibrant atmosphere. However, this time we could not publish any photograph. The photographs submitted for the issue, despite being technically sound, lack unique aesthetic message. We sincerely hope that the photographs would be of novel theme in the forthcoming issues.

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BOSE FEST 2014



Bose Fest showcased the spirit of creativity and science through a 2-day long festival held within the Center's premises during 30- 31 January 2014. All academic colleagues were invited for spontaneous participation in this yearly science celebration under SCOLP, EVLP. All students belonging to 3rd and 4th years delivered oral presentation, while the rest made poster presentations. All talks were of 15 (12 + 3) minutes duration. This year there were 38 Talks and 40 Posters presented by the students. The talk sessions were divided into four Sessions corresponding to the Departments at the Centre.

The program was inaugurated by Prof. A.K Raychaudhuri, Director at the Silver Jubilee Hall. The Condensed Matter Physics and Material Sciences session were chaired by Prof. Priya Mahadevan (SNBNBS), Dr. Sujit Bandyopadhyay (VECC, Kolkata), Dr. Manoranjan Kumar (SNBNBS), and Dr. D. Das (UGC DAEF, Kolkata). The Chemical, Biological and Macro-Molecular Sciences sessions were chaired by Prof. Tapas Chakraborty (IACS, Kolkata) and Prof. Pradip K.Ghorai (IISER- Kolkata). Prof. A.S. Majumder (SNBNCBS) chaired the session on Astrophysic & Cosmology. The session on Theoretical Sciences were chaired by Dr. Shraddha Mishra (SNBNBS), and Prof. Biswajit Chakraborty (SNBNBS).

All academic colleagues were encouraged to participate through poster presentations and intellectually stimulating discussions. Cultural performance by Muktagan followed by Family dinner was held on 30.01.14. The curtains fell with the Prize distribution ceremony for the best talk and Poster presentation by the Director on 31.01.14.

ACADEMIC REPORT

Coupled Magnetic Vortices for All-Magnetic Transistor Operations

Dheeraj Kumar, Saswati Barman, and Anjan Barman

Transistors constitute the backbone of modern day electronics. Since their advent, researchers have been seeking ways to make smaller and more efficient transistors. Recently, we demonstrated a sustained amplification of magnetic vortex core gyration in coupled two and three vortices by controlling their relative core polarities. This amplification is mediated by a cascade of antivortex solitons travelling through the dynamic stray field. We further demonstrated that the amplification can be controlled by switching the polarity of the middle vortex in a three vortex sequence and the gain can be controlled by the input signal amplitude. The above observations promote the magnetic vortices as suitable candidates to work as stable bipolar junction transistors.

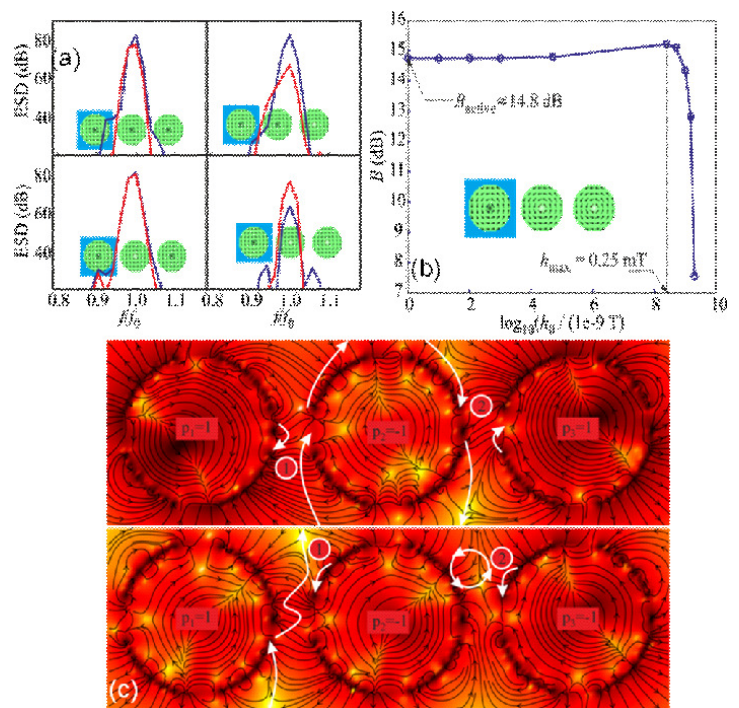
In laterally confined ferromagnetic nanodisks, isolated magnetic vortices can be formed, if it is energetically favourable. The central region with out of plane magnetization is called vortex core and it is only a few nanometres in diameter. The direction of out of plane magnetization in the core is termed as polarity and it can possess either of two highly discrete and mutually exclusive values: $p = 1$ or $p = -1$ depending upon the direction out of plane or into the plane. The direction of the in-plane curling magnetization is called chirality; and it is either in the clockwise (CW) or the counter-clockwise (CCW) flux closure configuration. Magnetic vortices can be brought to gyration by the application of the magnetic fields and spin polarized currents. We examined the potential of this gyration in terms of signal transduction and amplification. In the case of coupled pair of vortices, when an excitation signal is applied to only one of the vortex then in certain situations, considerably more energy is stored in its neighbouring vortex (signal amplification) if it has the opposite polarity. We further observed that this significant relative gain of gyrotropic amplitude can be extended over three vortices for a particular case of core polarity combination $(p_1, p_2, p_3) = (1, ?1, ?1)$. In Fig. 1 (a), we plot the energy spectral density (ESD) corresponding to the gyrotropic modes of left and right most vortices in different polarity configurations as shown in their insets. Here an amplification is seen only for $(p_1, p_2, p_3) = (1, ?1, ?1)$. However, this ceases to be the case if p_2 is switched from ?1 to 1. Thus, the two classic transistor operations of *signal switching* and *amplification* are realized with the help of magnetic vortices. We also examined the dependence of gain on signal amplitude as shown in Fig. 1 (b). We found that gain B , remains stable ($B = B_{\text{active}} = 14.8$ dB) for very low signal amplitudes mimicking the *active* state of an electronic transistor under small signal condition. The gain swiftly dropped after a signal amplitude of about 2.5 mT indicating a state of saturation. The *cut-off* state can be obtained by switching the polarity of the middle vortex. Thus we were able to demonstrate all three conventional operational states of an electronic transistor – *cut-off*, *active*, and *saturation* – by the help of magnetic vortices.

We have probed the origin of these interesting observations by using

the temporal evolution of stray magnetic field and observed that antivortex packets moving through the field were accountable for the observed amplifications (Fig. 1(c)). While attempting a fan-out of the signal to two symmetrically placed branches, we noticed that only one of the branches showed amplification while the other did not. It is due to the fact that solitons involved in the transfer of energy as topologically stable and they favour the branch which comes in their path first. We believe that further study of these solitons will aid the research community in creating a better analytical model, which can predict such useful results as signal amplification without the need to do complete simulations.

References

D. Kumar, S. Barman and A. Barman “Magnetic Vortex Based Transistor Operations”, *Scientific Reports* (Nature Publishing Group)



4, 4018 (2014).

Fig. 1. **Magnetic vortex transistor.** (a) Energy spectral densities (ESDs) of left and right magnetic vortices with different combinations of vortex core polarization in the three vortex sequence. A 1.5 mT signal rotating CCW at the resonant frequency is applied only to the left (shaded) vortex. (b) Gain B , versus logarithm of signal amplitude h_0 . (c) Magnetic stray field distribution in the cases where (p_1, p_2, p_3) equals $(1, -1, 1)$ (upper panel) and $(1, -1, -1)$ (lower panel). The path of anti-vortex packets after the dynamics has stabilized is marked with solid lines.

Best Poster Awards in Conferences From to the students of the Centre working with Anjan Barman

1. Arnab Ganguly from the lab of Anjan Barman won the best poster award in the DAE-BRNS Theme Meeting on Ultrafast Sciences (UFS-2013) at IIT Kharagpur during 25-26 Oct., 2013 for the paper:

“Time-Domain Magneto-Optical Kerr Effect Investigation of

EVENTS

Precessional Dynamics in Ion-Irradiated Transition-Metal Capped NiFe Thin Films” by A. Ganguly, S. Pal, J. A. King, D. A. Burn, A. T. Hindmarch, D. Atkinson, and A. Barman.

2. Semanti Pal from the same lab won the best poster award in the 58th Annual Magnetism and Magnetic Materials (MMM) conference at Denver Colorado, USA during 4-8 Nov., 2013 for the paper:

“Effect of the Spin Twist Structure on the Spin Wave Dynamics in $\text{Fe}_{55}\text{Pt}_{45}/\text{Ni}_{80}\text{Fe}_{20}$ Exchange Coupled Bi-layers with Varying $\text{Ni}_{80}\text{Fe}_{20}$ Thickness” by S. Pal, S. Barman, O. Hellwig, and A. Barman.

3. Susmita Saha from the same lab won the best poster award in MagMA-2013 at IIT Guwahati during 5-7 Dec., 2013 for the paper:

“Tunable and Anisotropic Spinwaves in Two-Dimensional Nanodot Lattices with Variable Lattice Symmetry” by S. Saha, R. Mandal, S. Barman, D. Kumar, B. Rana, and A. Barman.

4. Bipul K. Mahato from the same lab won the best poster award in MagMA-2013 at IIT Guwahati during 5-7 Dec., 2013 for the paper:

“Spin Wave Modes in Cross Shaped Magnetic Nanoelements” by B. K. Mahato, B. Rana, R. Mandal, D. Kumar, S. Barman, S. Sugimoto, Y. Fukuma, Y. Otani and A. Barman.

5. Debanjan Polley from the same lab won the best poster award in IUMRS-ICA 2013 at IISc Bangalore during 16-20 Dec., 2013 for the paper:

“THz Shielding Efficiency of Carbon Nanotubes in Polymer Film” by D. Polley, A. Barman and R. K. Mitra.

6. Ruma Mandal from the same lab won the best poster award in Physics and Chemistry of Materials : Computation and Experiments, S. N. Bose National Centre for Basic Sciences, 24-25 Feb. 2014 for the paper:

“Effects of Antidot Shape on the Spin Wave Spectra of Two-dimensional $\text{Ni}_{80}\text{Fe}_{20}$ Antidot Lattices” by R. Mandal, P. Laha, K. Das, S. Saha, S. Barman, A. K. Raychaudhuri and A. Barman.

7. Samapan Sikdar, joint student of Jaydeb Chakrabarti and Mahua Ghosh, won the D. M. Bose memorial award in Annual Conference of Indian Biophysical Society, Molecular Architecture, Dynamics and Assembly in Living Systems during Feb 7-10 at SINP, Kolkata for the poster:

“Thermodynamics of conformational changes upon metal ion binding to a metalloprotein” by Samapan Sikdar, J. Chakrabarti and Mahua Ghosh.

8. Suman Dutta, student of Jaydeb Chakrabarti, won the best poster award at CTBBM during 7-8 Oct, 2014 at SNBNCBS for the paper:

“Dynamics of self-organization in driven colloids”, Suman Dutta and J. Chakrabarti.

Report on Current Trends in Biochemical and Biophysical Modelling (CTBBM2013), 7-8th October, 2013

Mahua Ghosh

The activities in the area of biophysical and biochemical modelling and computation are gaining momentum with the advent of new theoretical and computational techniques. The main purpose of the meeting was to bring together people working in these areas and making a nation-wide network of such newly emerging research activities.

The meeting was organized by Jaydeb Chakrabarti, Gautam Gangopadhyay and Mahua Ghosh at the S. N. Bose National Centre for Basic Sciences with funding from the S. N. Bose Centre. A total of 18 talks and 21 posters were presented in the meeting. The speakers included young and vibrant scientist from all over the country, like Sudipta Maiti (TIFR, Mumbai), Sachi Gosavi (NCBS, Bangalore), Satyavani Vemparala (IMSc, Chennai), Pradipto Bandyopadhyay (JNU, New Delhi), Suman Banik (Bose Institute, Kolkata) and so on. There were 5 internal speakers highlighting the activities of the centre in the area of Biochemistry and Biophysics. The posters were presented by all other participants primarily consisting of young PhD students. The organizers covered the travel expenses of all the outstation participants (4 in number), although no travel support could be given to the outstation speakers (8 in number) due to limited budget. Three best poster awards (Rs. 5000/-, Rs. 3000/- and Rs.2000/-) were given according to the judgement of a jury board consisting of Ananda Mohan Ghosh (IISER, Kolkata), Suman Banik (Bose Institute, Kolkata), Sanjoy Bandyopadhyay (IIT Kharagpur), Sudipta Maiti (TIFR, Mumbai) and Prabal Maiti (IISc, Bangalore). N. M. Mascarenhas from NCBS got the first prize; Samapan Sikdar and Suman Dutta from the Centre bagged the 2nd and the 3rd prizes, respectively.

The Bose Test 2014

The Bose Test for the aspirants of PhD Programme in our Centre was held on 06.04.2014. The test was carried out in several Centres in Kolkata and other major cities including New Delhi, Chennai, Varanasi, Bangalore and so on. More than 1000 students (IPhD 620, PhD/Physical Sciences 431 and PhD/Chemical Sciences 256) all over the country appeared at this test. The final selections, however, are subject to minimum marks criterion and the interview held at a later date. This test is an important avenue for the chemistry students for admission to the PhD Programme in Chemical Sciences.

Fire Safety Management Course

Swarup Dutta

A continuing professional development programme on “Fire Safety Management Course” was organized by ‘International Institute of Security and Safety Management’ during 4th to 5th March 2014 in the Centre. Staffs from SNBNCBS attended the training programme. The course consisted of Fire Safety related issues including the Safety Setup, Statutory Compliances & Challenges in West Bengal including few case studies, like AMRI Hospital Fire Incident.

Training on Noting, Drafting & Office Management

Shobini Majumder

The Centre has organized a two-day training programme on 'Noting, Drafting & Office Management' during 29-30 April and 1-2 May 2014. The programme was conducted by IISWBM. It was conducted in two batches, comprising of 52 (Fifty Two) administrative and 7 (Seven) academic staff members. The programme comprised of interactive sessions on topics like Noting, Drafting, function of receiving and despatch section, record management, few aspects of financial management, HR Interphase etc.

Training on Basic Life Support (BLS) and First Aid

Siddhartha Chatterjee

The Centre organised a training on Basic Life Support (BLS) and First Aid on 21st March 2014 at Silver Jubilee Hall. The training was conducted by doctors and experts of Apollo Gleneagles Hospitals, Kolkata. The axiom of the training was to impart knowledge on Basic Life Saving and First Aid support for handling any trauma during emergency conditions.

FROM THE DEAN (ACADEMIC PROGRAMME)'S DESK

Ph.D. AWARDS

Theoretical Studies on the Nonadiabatic effects in Molecular Aggregates, Kinshuk Banerjee, Supervisor: Gautam Gangopadhyay, in University of Calcutta, on May 17, 2013

Study of Electronic Structure of Disordered Systems, Prashant Singh, Supervisor: Abhijit Mookerjee, University of Calcutta, on June 7, 2013

Stochastic approaches to heterogeneous and complex reaction kinetics, Biswajit Das, Supervisor: Gautam Gangopadhyay, in University of Calcutta, on June 24, 2013

Pairing and Condensation in Ultracold Quantum Gases, Raka Dasgupta, Supervisor: Jayanta K Bhattacharjee, in Jadavpur University, on June 27, 2013

Heat Transport and Related Thermal Properties in Nanofluids and Nanostructured Materials, Rajesh Kumar Neogy, Supervisor: Arup K Raychaudhuri, in Jadavpur University, on June 27, 2013

Numerical Simulation of Viscous Accretion Flows around Black Holes which include Shocks, Kinsuk Giri, Supervisor: Sandip K Chakrabarti, in Jadavpur University, on June 27, 2013

First Principles Study of Silicate Minerals, Swastika Chatterjee, Supervisor: Tanusri Saha Dasgupta, in University of Calcutta, on August 2, 2013

Studies on Biomolecular Recognition Using Ultrafast Laser Spectroscopic Techniques, Tanumoy Mondol, Supervisor: Samir Kumar Pal, in University of Calcutta, on September 17, 2013

Study of Nanostructured Iron Oxides, Arka Chaudhuri, Supervisor: Kalyan Mandal, in University of Calcutta, on October 3, 2013

Electronic, Magnetic and Structural Properties of Transition Metal Oxides, Kapil Gupta, Supervisor: Priya Mahadevan, in Jadavpur

University, on October 8, 2013

First Principle study of Novel Materials, Sudipta Kanungo, Supervisor: Tanusri Saha Dasgupta, in University of Calcutta, on December 5, 2013

Electronic and Magnetic Properties of Systems without Periodicity, Rudra Banerjee, Supervisor: Abhijit Mookerjee, in University of Calcutta, on December 11, 2013

Spectroscopic Studies of Molten Electrolyte Mixtures, Binary Polar Solvent Mixtures and Solvents under Confinement, Biswajit Guchhait, Supervisor: Ranjit Biswas, in Jadavpur University, on December 2013

Spectroscopic Studies on Photoreactivity of Inorganic Nanocrystals and Medicinally Important Organic Dyes, Soumik Sarkar, Supervisor: Samir Kumar Pal, in Jadavpur University, on December 2013

Numerical Modeling of VLF Radio Wave Propagation through Earth-Ionosphere Wave guide and its application to Sudden Ionospheric Disturbances, Sujay Pal, Supervisor: Sandip K Chakrabarti, in University of Calcutta, on January 2, 2014

Phase Transition in Black Holes, Dibakar Roychowdhury, Supervisor: Rabin Banerjee, in University of Calcutta, on January 7, 2014

Dynamics of Neat Ionic Liquid, Binary mixtures and Liquids under Confinement: Theoretical and Simulation study, Snehasis Daschakraborty, Supervisor: Ranjit Biswas, in Jadavpur University, on February 20, 2014

A Study of Certain Properties of Nonlinear Ordinary Differential Equations, Barun Khanra, Supervisors: Partha Guha & Anindya Ghose Choudhury (Surendranath College), in West Bengal State University, on February 21, 2014

Study of Planar models in Quantum Mechanics, Field theory and Gravity, Sarmishtha Kumar, Supervisor: Rabin Banerjee, in University of Calcutta, on March 26, 2014

Synthesis and Characterization of Multifunctional Nanoparticles and their Interaction with Biological Macromolecules, Anupam Giri, Supervisor: Samir Kumar Pal, in Jadavpur University, on March 26, 2014

Prepotential Formulation of Lattice Gauge Theories, Indrakshi Raychowdhury, Supervisor: Manu Mathur, in University of Calcutta, on April 4, 2014

THESIS REPORT

"Synthesis and Characterization of Multifunctional Nanoparticles and their Interaction with Biological Macromolecules"

Anupam Giri

Supervisor: Dr. Samir Kumar Pal, Dept. of Chemical, Biological & Macro-Molecular Sciences

The development of multifunctional nanoparticles with precise biological/chemical functions having economic, healthcare and environmental benefits are a key focus in nanobiotechnology and could

have profound impact on many research areas, ranging from molecular imaging to medical diagnostics /therapeutics, chemical conversion and energy production. Several novel nanomaterials have recently been described for their unique optical, magnetic, electronic and structural properties. Considerable efforts have also been directed towards rational surface modifications to modulate their complicated surface chemistry, high-specificity and efficient targeting. However, despite recent advancement, much works still need to be done in order to achieve: (i) hydrophilic and biocompatible NPs that are intrinsically luminescent, with surface chemistry adaptable to varied biological/chemical applications; (ii) selective and specific labeling of live cells and biomolecules.

In the present thesis, we have explored a molecular functionalization strategy to solubilize one of the promising manganite nanoparticles $\text{La}_{0.67}\text{Sr}_{0.33}\text{MnO}_3$ (LSMO) in aqueous environments. The electronic structural modification of the NPs imparted through functionalization and subsequent water solubilization reveals multiple absorption bands in the UV-vis region. Using the absorption band of the functionalized NPs we have monitored their interaction with other biologically important ligands such as 4-nitrophenylanthranilate (NPA) and a DNA base mimic, 2-aminopurine (2AP). Förster resonance energy transfer (FRET) of the covalently attached probe NPA with the capped NPs confirm their attachment with the surface functional group ($-\text{OH}$) of the citrate ligand, whereas, the FRET of 2AP, with the NPs confirm the surface adsorption of the 2AP molecules. Further treatment of the solubilized NPs, lead to the emergences of multi-color photoluminescence (from blue to red region of the spectrum) when it is addressed with different excitation wavelengths, where the respective excitation wavelengths have a direct correlation with the observed UV-vis absorption bands. Using a multitude of spectroscopic tools we have investigated the mechanistic insight behind the origin of different absorption bands and emergence of multicolor photoluminescence from the functionalized NPs. Moreover, using Mn_3O_4 NPs we demonstrate their surface modification induced multiple photoluminescence and room temperature ferromagnetic activation. Moreover, employing a systematic variation of the ligands, their functional groups and the structural position of the functional groups, we have identified the necessary and sufficient structural requirement of the surface co-ordinating ligands, to induce such unprecedented optical/magnetic responses from the NPs. In this direction, we have exchanged TOPO (trioctylphosphine oxide) ligand of CdSe/ZnS core/shell quantum dots (QDs) with an amino acid L-arginine (Arg) at the toluene/water interface and eventually rendered the QDs from toluene to aqueous phase. We have studied the interaction of the water soluble Arg-capped QDs (energy donor) with ethidium (EB) labeled synthetic dodecamer DNA (energy acceptor) using picoseconds resolved FRET technique.

Apart from the fundamental scientific interest, these results represent a promising route for surface modification mediated rational designing of NPs adaptable to diverse applications and a logical extension of these works would be the functionalization of various manganese doped nanoparticles and QDs.

List of Publication:

1. **A. Giri**, A. Makhal, B. Ghosh, A. K. Raychaudhuri and S. K. Pal “Functionalization of manganite nanoparticles and their interaction with biologically relevant small ligands: Picosecond time-resolved FRET studies”, *Nanoscale*, 2010, 2, 2704–2709
2. **A. Giri**, N. Goswami, M. S. Bootharaju, P. L. Xavier, R. John, N. T. K. Thanh, T. Pradeep, B. Ghosh, A. K. Raychaudhuri, S. K. Pal: “Emergence of Multicolor Photoluminescence in $\text{La}_{0.67}\text{Sr}_{0.33}\text{MnO}_3$ Nanoparticles” *Journal of Physical Chemistry C*, 116 (2012) 25623.
3. **A. Giri**, N. Goswami, M. Pal, MTZ. Myint, S. Al-Harhi, A. Singha, B. Ghosh, J. Dutta and S. K. Pal: “Rational Surface Modification of Mn_3O_4 Nanoparticles to Induce Multiple Photoluminescence and Room Temperature Ferromagnetism” *Journal of Materials Chemistry C* 1 (2013) 1885.
4. **A. Giri**, N. Goswami, P. Lemmens and S. K. Pal “Preparation of water soluble L-arginine capped CdSe/Zns QDs and their interaction with synthetic DNA: Picosecond-resolved FRET study”, *Materials Research Bulletin* 47 (2012) 1912 (Cover Article).
5. **A. Giri**, N. Goswami, S. Sarkar, and S. K. Pal “Bio-Nanomaterials: Understanding Key Biophysics and their Applications”, (Book Chapter) in “Biomaterials” Edited by J.N. Govil, STUDIUM PRESS LLC, USA, 2013.
6. N. Goswami, **A. Giri**, M. S. Bootharaju, P. L. Xavier, T. Pradeep and S. K. Pal “Copper Quantum Clusters in Protein Matrix: Potential Sensor of Pb^{2+} ion”, *Analytical Chemistry*, 83 (2011) 9676.
7. N. Goswami, **A. Giri**, S. Kar, M. S. Bootharaju, R. John, P. L. Xavier, T. Pradeep and S. K. Pal “Protein directed synthesis of NIR-emitting, tunable HgS quantum dots and their applications in metal ion sensing”, *Small* 8 (2012) 3175.
8. N. Goswami, **A. Giri**, and S. K. Pal: “ MoS_2 Nanocrystals Confined in DNA Exhibiting Energy Transfer” *Langmuir* (2013) In Press.
9. P. K. Verma, **A. Giri**, N. T. K. Thanh, L. D. Tung, O. Mondal, M. Pal and S. K. Pal “Superparamagnetic fluorescent nickel-enzyme nanobioconjugates: synthesis and characterization of a novel multifunctional biological probe”, *Journal of Materials Chemistry*, 2010, 20, 3722–3728.

Patent:

1. Giri et al. “Tartrate Functionalized LSMO Nanoparticles, its manner of manufacture and Biomedical probe”; Indian Pat. Appl. (2011), 979/KOL/2011 dated 25th July 2011.

“Investigations of complex systems: from Granular to cognitive systems”

Dattatreya P Shinde

Supervisor: Professor Anita Mehta, Department of Theoretical Sciences

We investigate the dynamics of granular spheres and human eye movements. In an experiment involving semantic search, the visual movements of sample populations subjected to visual and aural input

were tracked in a taskless paradigm. The probability distributions of saccades and fixations were obtained and analyzed. Scale-invariance was observed in the saccadic distributions, while the fixation distributions revealed the presence of a characteristic (attentional) time scale for literate subjects. Levy random walks effectively describe the super-diffusive dynamics of searching behavior. We constructed two dimensional ordinary Levy random walk model for eye movements. This model has been validated for super-diffusive dynamics by comparison with both experimental and numerical results. A detailed analysis of our results suggests that saccadic eye motions are an example of Levy, rather than Brownian, dynamics. We applied likelihood and Akaike information techniques to experimental and simulated data. Power law distribution has maximum likelihood and Akaike weights against Gamma and Exponential distributions. These statistical techniques effectively select the best fitting model for the data from the set.

We use a hybrid Monte Carlo algorithm to simulate the shaking of spheres at different vibration amplitudes, and find that spontaneous crystallization occurs in specific dynamical regimes. Several crystallizing transitions are typically observed, leading to end states which can be fully or partially ordered, depending on the shaking amplitude, which we investigate using metrics of global and local order. At the lowest amplitudes, crystallization is incomplete, at least for our times of observation. For amplitude ranges where crystallization is complete, there is typically a competition between hexagonal close packed (hcp) and face-centered cubic (fcc) ordering. It is seen that fcc ordering typically predominates; in fact for an optimal range of amplitudes, spontaneous crystallization into a pure fcc state is observed. An interesting feature is the breakdown of global order when there is juxtaposition of fully developed hcp and fcc order locally: we suggest that this is due to the interfaces between the different domains of order, which play the same role as dislocations. Delaunay tessellations give structural insights of granular packing at various densities. We described a statistical mechanics of local volumes and entropies of tessellation simplexes. Taken together, findings of local volumes highlighted that the fluctuations, entropies have shown drastic change at packing densities 0.62, 0.64 and 0.68. The length and angular measures of tessellation provides a basis for distinguishing crystalline structures. We computed edges and their lengths, length measures tetrahedrality and quartohedrality, and dihedral angle distributions of tessellations. Minima's of length measures and distributions of edge, and dihedral angles clearly separate the regularity of tessellation simplexes.

Publications

1. D. P. Shinde, Anita Mehta and R. K. Mishra, *Europhys. Lett.* **94**, 68001 (2011).
2. D. P. Shinde, Anita Mehta and G. C. Barker, *Phys. Rev. E* **89**, 022204 (2014).
3. D.P. Shinde (In Preparation)
4. D.P. Shinde (In Preparation)

"Effects of curvature and gravity from flat spacetime"

Debraj Roy

Supervisor: Professor Rabin Banerjee, Department of Theoretical Sciences

The equivalence principle played a fundamental role in formulating the theory of general relativity. It investigates the relationship between different frames of references, in particular, emphasising the role of accelerated frames in understanding gravity. We adopt this as a preamble and investigate two lines of thought. In one, we study the role of the accelerated observer's horizon while he sees quantum fields and vacua - to study the Unruh effect. Here, an accelerated observer sees the empty Minkowski space as a thermal background with a black-body spectrum, characterised by a specific temperature. We adopt the methodology of quantum tunneling (which is simpler than the typical field theoretic approach) to derive the Unruh temperature and spectrum. This effect is closely related to the Hawking effect in black holes, the bridge being the principle of equivalence. In another direction, we try to (in a sense) recover the equivalence principle, starting from the gauge principle. Gauge symmetries have been pivotal to our understanding of fundamental interactions. Our known world (particles) is described by the 'standard model' having certain internal gauge symmetries, along with global Poincare symmetries. Localising these Poincare symmetries give rise to a formulation of gravity, known as the Utiyama-Kibble-Sciama 'Poincare gauge theory.' This theory has the (local) Poincare symmetries inbuilt. We resolve certain interesting puzzles related to classical gauge symmetries in the models, using rigorous methods suitable for such constrained hamiltonian systems.

References

- [1] Rabin Banerjee and Roy, Debraj. "Trivial gauge transformations in Poincare gauge gravity". Written for proceedings of 13th Marcel Grossmann Meeting (MG13), Stockholm, Sweden, 1-7 July 2012.
- [2] Roy, Debraj. "Lagrangian analysis of 'trivial' symmetries in models of gravity". Accepted for publication in the proceedings of the meeting 'Relativity and Gravitation, 100 Years after Einstein in Prague,' held in Prague, Czech Republic during June 25 - 29, 2012.
- [3] Rabin Banerjee and Roy, Debraj. "Trivial symmetries in a 3D topological torsion model of gravity". *J.Phys.Conf.Ser.*, 405:012028, 2012.
- [4] Rabin Banerjee and Roy, Debraj. "Poincare gauge symmetries, hamiltonian symmetries and trivial gauge transformations". *Phys.Rev.*, D84:124034, 2011.
- [5] Rabin Banerjee, Sunandan Gangopadhyay, and Roy, Debraj. "Hamiltonian analysis of symmetries in a massive theory of gravity". *JHEP*, 1110:121, 2011.
- [6] Rabin Banerjee, Roy, Debraj, and Saurav Samanta. "Lagrangian generators of the Poincare gauge symmetries". *Phys.Rev.*, D82:044012, 2010.
- [7] Rabin Banerjee, Sunandan Gangopadhyay, Pradip Mukherjee, and Roy, Debraj. "Symmetries of topological gravity with torsion in the hamiltonian and lagrangian formalisms". *JHEP*, 1002:075, 2010.
- [8] Roy, Debraj. "The Unruh thermal spectrum through scalar and fermion tunneling". *Phys.Lett.*, B681:185-189, 2009.

“Development of Nanoscale Systems for Spin-Wave Propagation”

Dheeraj Kumar

Supervisor: Professor Anjan Barman, Department of Condensed Matter Physics and Material Sciences

It has been proposed that spin-waves, particularly those with frequencies in microwave and submillimeter wave bands, can be used for information transmission and processing. Having shorter wavelengths as compared to electromagnetic waves of the same frequency, spin-wave based devices hold the potential to aid the miniaturization of microwave communication. Designs have been proposed which use nanoscale magnetic systems to create elements which can function as attenuators, filters, phase-shifters, interferometers and logic gates. Here, we study the magnetization dynamics of spin-wave dispersion and magnetic vortex gyration. Both phenomenon are related and have their characteristic frequencies in the microwave frequency band. The nanoscale systems considered here are ferromagnetic thin films, uniform waveguides, magnonic crystals (spatially modulated magnetic systems) and magnetic vortices. Effects like magnetization pinning and mirror symmetry breaking, which alter the spin-wave dispersion characteristic call for greater spatial resolution and precision in fabrication. Thus, we summarize with what needs to be done and the future directions the research needs to take in order to make nanoscale devices technically feasible.

The spectrum of spin-waves propagating in magnetic systems is important from both fundamental and applied points of views. Propagating spin-waves in magnonic crystals will form the building blocks of future microwave data processing and communication. While magnonic modes and band gaps can help in the formulation of filters and attenuators, understanding other phenomena like spin-wave reflection, refraction and interference will help in designing magnonic circuit elements like logic gates and diodes.

The Landau–Lifshitz–Gilbert (LLG) equation has been used in this work to simulate the spin dynamics in different nanoscale magnetic systems. This equation was solved mainly using the finite difference method based Object–Oriented Micromagnetic Framework (OOMMF) or the finite element method based Nmag. In addition to using some existing software packages, we also developed our own LLG equation solver (which can also take spin-transfer-torque terms into account) using MATLAB programming. The combined packages of simulation and post-processing has been named DotMag. DotMag can simulate spin dynamics in two-dimensional systems and can analyse results for any kind of nanoscale system — even those solved using third party packages, such as OOMMF. The results obtained from the newly developed software have been inspected for any magnonic bands and bandgaps using multi-domain discrete Fourier transform. Various issues related to the numerical calculations like aliasing, spectral leakage and scalloping loss have been addressed in Chap. 3. The tools prepared for analysing these magnonic conductors will also allow for the visualization of propagation and power and phase distribution of the spin-wave over the entire region of interest. These tools will be generically designed, so as to accommodate any kind of magnonic conductor.

The newly developed package DotMag was used for the calculations

of magnonic band structures of one- and two-dimensional periodic arrays of dots, anti-dots (holes created in continuous magnetic medium) and filled antidots (the holes are now filled with a different magnetic medium). Influence of different structural and material parameters over the spin-wave band structure was studied in these cases. The results obtained using the micromagnetic simulations were also compared with those obtained from the plane wave method (PWM) and any differences were examined. Iso-frequency lines, which are magnonic analogues of the electronic Fermi surfaces were also calculated in the case of two-dimensional antidot arrays. With the knowledge obtained from above we investigated magnonic waveguides embedded with regular and filled antidots to design magnonic filters of tunable bandwidth and bandgaps. Some of the numerically examined magnonic crystals have been fabricated by using different lithography techniques. The low wavevector magnonic modes in some of these magnonic crystals were experimentally investigated by using our TR-MOKE experimental setup.

In Chap. 5, we study the spin-wave spectra in magnonic antidot waveguides (MAWs) versus the surface anisotropy at the ferromagnet/air interface. The MAWs under investigation have the form of a thin stripe of permalloy with a single row of periodically arranged antidots in the middle. The introduction of a magnetization pinning at the edges of the permalloy stripe and the edges of antidots is found to modify quantitatively the spin-wave spectrum. This effect is shown to be necessary for magnonic gaps to open in the considered systems. Our study demonstrates that the surface anisotropy can be crucial in the practical applications of MAWs and related structures and in the interpretation of experimental results in one- and two-dimensional magnonic crystals. We used three different theoretical methods i.e. PWM, finite difference method and finite element method to validate the results. We showed that PWM in the present formulation assumes pinned magnetization while in micromagnetic simulations special care must be taken to introduce pinning.

In Chap. 6, we theoretically study the spin-wave spectra in magnonic waveguides periodically patterned with nanoscale square antidots and show that structural changes breaking the mirror symmetry of the waveguide can close the magnonic bandgap. But, the effect of these intrinsic symmetry breaking factors can be compensated by a properly adjusted asymmetric external bias magnetic field, i.e., by an extrinsic factor. This allows for the recovery of the magnonic bandgaps occurring in the ideal symmetric structure. The described methods can be used for developing parallel models for recovering bandgaps closed due to an intrinsic defect, e.g. a fabrication defect. The theoretical model developed here is particular to the field of magnonics, a rapidly emerging field combining spin dynamics and spintronics. However, the underlying principle of this development is squarely based upon the translational and mirror symmetries associated with a regular crystal structure. Thus, we believe that this idea of correcting an intrinsic defect by extrinsic means, should be applicable to spin-waves in both exchange and dipolar interaction regimes, as well as to electron, electromagnetic and acoustic waves in general.

In Chap. 7, we present the possibility of tuning the spin-wave band structure, particularly the bandgaps in a nanoscale magnonic antidot waveguide by varying the shape of the antidots. The effects of changing the shape of the antidots on the spin-wave dispersion

relation in a waveguide have been carefully monitored. We interpret the observed variations by analysing the equilibrium magnetic configuration and the magnonic power and phase distribution profiles during spin-wave dynamics. The inhomogeneity in the exchange fields at the antidot boundaries within the waveguide is found to play a crucial role in controlling the band structure at the discussed length scales. The observations recorded here will be important for future developments of magnetic antidot based magnonic crystals and waveguides.

In Chap. 8, we demonstrate that the magnonic band structure, including the band gap of a ferromagnetic antidot waveguide, can be significantly tuned by a relatively weak modulation of its structural parameters. We study the magnonic band structure in nanoscale spin-wave waveguides with periodically distributed small antidots along their central line by two independent computational methods, namely, a micromagnetic simulation and a plane-wave method. The calculations were performed with consideration of both the exchange and dipolar interactions. For the exchange dominated regime, we discuss, in details, the impact of the changes of the lattice constant, size, and shape of the antidots on the spin-wave spectra. We have shown that a precise choice of these parameters is crucial for achieving desired properties of antidot waveguides, i.e., a large group velocity and filtering properties due to existence of magnonic band gaps. We discuss different mechanisms of magnonic gap opening resulting from Bragg scattering or anticrossing of modes. We have shown that the dipolar interactions start to assert their role in the spin-wave spectrum when the waveguide is scaled up, but even for a period of few hundreds of nanometres, the magnonic band structure preserves qualitatively the properties found in the exchange dominating regime. The obtained results are important for future development of magnonic crystal based devices.

In Chap. 9, we present the observation of a complete bandgap and collective spin-wave excitation in two-dimensional magnonic crystals comprised of arrays of nanoscale antidots and nanodots, respectively. Considering that the frequencies dealt with here fall in the microwave band, these findings can be used for the development of suitable magnonic metamaterials and spin-wave based signal processing. We also present the application of a numerical procedure, to compute the dispersion relations of spin-waves for any high symmetry direction in the first Brillouin zone. The results obtained from this procedure has been reproduced and verified by the well-established PWM for an antidot lattice, when magnetization dynamics at antidot boundaries is pinned. The micromagnetic simulation based method can also be used to obtain iso-frequency contours of spin-waves. Iso-frequency contours are analogous of the Fermi surfaces and hence, they have the potential to radicalise our understanding of spin-wave dynamics. The physical origin of bands, partial and full magnonic bandgaps has been explained by plotting the spatial distribution of spin-wave energy spectral density. Although, unfettered by rigid assumptions and approximations, which afflict most analytical methods used in the study of spin-wave dynamics, micromagnetic simulations tend to be computationally demanding. Thus, the observation of collective spin-wave excitation in the case of nanodot arrays, which can obviate the need to perform simulations may also prove to be valuable.

DotMag was developed with the ability to excite vortex core gyration by using external magnetic field and spin transfer torque. Magnetic vortex dynamics was investigated in the cases of isolated and coupled vortices. Transducer and transistor like operations were demonstrated based on these results. Transistors constitute the backbone of modern day electronics. Since their advent, researchers have been seeking ways to make smaller and more efficient transistors. In Chap. 12, we demonstrate a sustained amplification of magnetic vortex core gyration in coupled two and three vortices by controlling their relative core polarities. This amplification is mediated by a cascade of antivortex solitons travelling through the dynamic stray field. We further demonstrated that the amplification can be controlled by switching the polarity of the middle vortex in a three vortex sequence and the gain can be controlled by the input signal amplitude. An attempt to show fan-out operation yielded gain for one of the symmetrically placed branches which can be reversed by switching the core polarity of all vortices in the network. The above observations promote the magnetic vortices as suitable candidates to work as stable bipolar junction transistors (BJT).

“Spectroscopic Studies on the Interactions of Biomimetics with Biological Macromolecules”

Ranajay Saha

Supervisor: Dr. Samir Kumar Pal, Department of Chemical, Biological & Macro-Molecular Sciences

Studies in dilute solution have yielded essential information about the biophysical properties of macromolecules like proteins. However, the cellular milieu is rich in diversity of both simple and complex molecules, and also quite crowded. For example, in *E. coli*, the cytoplasm is estimated to contain 300-400 mg/mL of proteins, nucleic acids, and various small molecules. The complex milieu inside cells can change these properties. Studying the nature and magnitude of these changes should improve our understanding of how biological macromolecules function in their native environments. A type of crowding called confinement refers to situations in which macromolecules find themselves inside small compartments. Confining proteins or in general biomacromolecules inside artificially created hosts is an effective approach for mimicking living cells. Accordingly, proteins can be suitably confined in a variety of inorganic, organic, and even inorganic-organic hybrid matrixes. Surfactant based vesicles, reverse micelles (RM), and various cyclic oligosaccharides etc. have been a convenient choice for similar studies. The present research includes study on the crucial ultrafast dynamical events in biomimetic self-assembly. In our study conventional organic chromophores have been employed to unravel picosecond-resolved solvation dynamics of water in biomimicking systems like microemulsions, vesicles and reverse vesicles [3, 9, 11]. The present works also explores the drug delivery potentiality of the biomimicking systems [11]. The *in vitro* dialysis experiments show the sustained release of therapeutic drugs from biomimicking AOT vesicles. In one of our study we provide the first proof-of-concept for the ability of reverse vesicular structures to be template of synthesizing metal nanoparticles (NPs) [3]. The as-prepared NP clusters are evaluated to be potential substrate for surface enhanced Raman Scattering (SERS) in solution [3].

Numerous biological processes involve electron transfer (ET) reactions and is crucial to life. In one of our study using femto- and picosecond resolved fluorescence spectroscopy, we capture the fast dynamics of the ET process and explore the nature of the specific ground and excited states that participate in the ET process leading to the photoconversion [2]. In another aspect of our study, we investigate how hydration and surface charge of the confinement, effect the ultrafast ET dynamics of riboflavin binding protein (RBP) to the bound cofactor riboflavin (Rf, vitamin B2), an important metabolic process, in nanoscopic AOT and CTAB RMs of various hydrations [6]. Visualization of the *in vitro* complex cellular processes involving proteins requires the use of spectroscopically distinguishable fluorescent reporters often realized by labelling of the protein. In one of our study we address the consequence of attachment of a fluoroprobe at the protein surface, in the molecular recognition of a model globular protein apomyoglobin by selectively small model receptor cyclodextrin of various cavity sizes [1]. A detailed study using both steady state and picosecond-resolved fluorescence spectroscopy illustrates the detrimental effect of hydrophobic fluorescent labels for proteins in biochemical studies involving recognition of molecules [1].

List of Publications

1. R. Saha, S. Rakshit and S. K. Pal "Molecular Recognition of a Model Globular Protein Apomyoglobin by Synthetic Receptor Cyclodextrin: Effect of Fluorescence Modification of the Protein and Cavity Size of the Receptor in the Interaction", *J. Molecular Recognition* (2013) DOI: 10.1002/jmr.2301.
2. R. Saha, P. K. Verma, S. Rakshit, S. Saha, S. Mayor and S. K. Pal "Light Driven Ultrafast Electron Transfer in Oxidative Redding of Green Fluorescent Proteins", *Sci. Rep.* 3 (2013) 1580.
3. R. Saha, S. Rakshit, D. Majumdar, A. Singha, R. K. Mitra, and S. K. Pal "Nanostructure, Solvation Dynamics and Nanotemplating of Plasmonically Active SERS Substrate in Reverse Vesicles", *J. Nanoparticle Res.* 15 (2013) 1576.
4. S. Rakshit, R. Saha, A. Singha, Zaki S. A. Seddigi and S. K. Pal "Molecular Interaction, Co-solubilisation of Organic Pollutants and Ecotoxicity of a Potential Carcinogenic Fuel Additive MTBE in Water" *J. Mol. Liquids* 180 (2013) 235.
5. S. Rakshit, R. Saha, A. Chakraborty and S. K. Pal "Effect of Hydrophobic Interaction on Structure, Dynamics and Reactivity of Water" *Langmuir* 29 (2013) 1808.
6. R. Saha, S. Rakshit, P. K. Verma, R. K. Mitra and S. K. Pal, "Protein-Cofactor Binding and Ultrafast Electron Transfer in Riboflavin Binding Protein under the Spatial Confinement of Nanoscopic Reverse Micelles" *J. Molecular Recognition* 26 (2013) 59.
7. S. Rakshit, R. Saha, P. K. Verma, R. K. Mitra and S. K. Pal, "Ultrafast Electron Transfer in Riboflavin Binding Protein in Macromolecular Crowding of Nano-Sized Micelle" *Biochimie* 94 (2012) 2673.
8. S. Rakshit, R. Saha, P. K. Verma and S. K. Pal, "Role of Solvation

Dynamics in Excited State Proton Transfer of 1-Naphthol in Nanoscopic Water Clusters Formed in a Hydrophobic Solvent" *Photochem. Photobiol.* 88 (2012) 851.

9. R. Saha, S. Rakshit, R. K. Mitra and S. K. Pal, "Microstructure, Morphology and Ultrafast Dynamics of a Novel Edible Microemulsion" *Langmuir* 28 (2012) 8309.
10. N. Goswami, R. Saha, S. K. Pal "Protein-assisted Synthesis Route of Metal Nanoparticles: Exploration of Key Chemistry of the Biomolecule" *J. Nanoparticle Res.* 13 (2011) 5485.
11. R. Saha, P. K. Verma, R. K. Mitra and S. K. Pal "Structural and Dynamical Characterization of Unilamellar AOT Vesicles in Aqueous Solutions and their Efficacy as Potential Drug Delivery Vehicle" *Colloids Surf., B.* 88 (2011) 345.
12. P. K. Verma, R. Saha, R. K. Mitra and S. K. Pal "Slow Water Dynamics at the Surface of Macromolecular Assemblies of Different Morphologies" *Soft Matter* 6 (2010) 5971.

"Spectroscopic Studies on the Biomolecular Recognition of Medicinally Important Ligands"

Soma Banerjee

Supervisor: Professor Samir Kumar Pal, Department of Chemical, Biological & Macro-Molecular Sciences

Biomolecular recognition is vital to cellular processes intervened by the formation of complexes between biomolecular receptors and their ligands. Proper understanding of biomolecular recognition is one of the most essential issues in modern molecular biology and has direct application in drug discovery and design. For example, exploration of the biomolecular recognition of some mutagens or carcinogens by DNA can highlight the pathways which can be targeted by some drugs to prevent the consequent mutation or carcinogenesis. On the other hand, the use of plants for medicinal purpose is probably as old as the history of mankind. Its use in the industrialized societies has led to the extraction and development of several alkaloids/drugs from plants. Therefore, upon exploring the biomolecular recognition of some mutagens and carcinogens by DNA, the basic insights into the role of plant alkaloids on such biomolecular recognition would be imperative for the practical utilization of such alkaloids as drugs. In view of the fact that binding involves solvent release from the binding site, the exploration of the behavior of water molecules associated with a biomolecular target or any other molecule which can regulate the biomolecular recognition is of significant interest. Besides, such biomolecular recognition is often associated with conformational changes involving both binding and folding. In this regard, spectroscopy has evolved as an efficient tool for the exploration of the dynamics of solvent molecules associated with biomolecules, ligands/biomolecular targets along with the changes associated with the binding and release of such ligands from the biological macromolecules.

The key focus of this thesis is to explore the photophysical properties of the medicinally important ligands using steady-state and time resolved fluorescence spectroscopic techniques for the fundamental understanding of their biomolecular recognition. For example, we have explored the structural evolution of caffeine self-aggregation

with temperature, since caffeine is consumed as low and high temperature beverages. Besides, we have investigated femtosecond-resolved dynamics of aqueous solvation within self-assembled dimeric structure of caffeine molecules employing fluorescent hydrophobic ligands like 4-(dicyanomethylene)-2-methyl-6-(p-methylaminostyryl)-4H-pyran (DCM) and coumarin 500 (C500). In addition, we have also focused on the consequence of the retarded dynamics of solvation on the photo-induced electron transfer (ET) or charge transfer (CT) reaction of a model probe, 2-(p-toluidino) naphthalene-6-sulfonate (TNS) encapsulated in the caffeine dimer. By employing picosecond resolved Förster resonance energy transfer (FRET) studies between a DNA minor groove binder dye Hoeschst 33258 (H258, donor) and ethidium (Et, acceptor), a model DNA-intercalator as well as a potential mutagen, the efficacy of caffeine in dissociating Et molecule from nanometer sized biomimicking micelles of different charges (cationic hexadecyltrimethylammonium bromide (CTAB), neutral (polar) Triton X-100 (TX-100) and anionic sodium dodecyl sulfate (SDS)) have been explored. In addition, systematic investigation on caffeine induced dissociation of Et molecule from various synthetic DNA *in-vitro*, and various cell lines in *ex-vivo* conditions has also been reported in one of our works. In another study we have emphasized UVA radiation induced ET reaction as one of the key aspects of a potential carcinogen, benzo[a]pyrene (BP) in the presence of a wide variety of molecules covering organic para-benzoquinone (BQ), biological macromolecules like calf-thymus DNA (CT-DNA), human serum albumin (HSA) protein and inorganic zinc oxide (ZnO) nanorods (NRs). We have also revealed the importance of the consideration of differential spectral overlap of the vibronic bands of BP undergoing FRET as a consequence of dipole-dipole interaction with an organic molecule in a biologically relevant confined environment. The experimental tools used for exploring the biomolecular recognition involve femto- and picosecond-resolved solvent relaxation dynamics. The different experimental techniques employed for the structural and functional characterization of the biomolecules include steady state UV-vis absorption and fluorescence, picosecond resolved fluorescence spectroscopy, Fourier transform infrared spectroscopy (FTIR), NMR spectroscopy, circular dichroism (CD), dynamic light scattering (DLS), fluorescence microscopy and scanning electron microscopy (SEM).

Publications

1. S. Banerjee, P. K. Verma, R. K. Mitra, G. Basu and S. K. Pal "Probing the Interior of Self-Assembled Caffeine Dimer at Various Temperatures", J. Fluorescence, 22 (2012) 753.
2. S. Banerjee, M. Tachiya and S. K. Pal "Caffeine Mediated Detachment of Mutagenic Ethidium from Various Nanoscopic Micelle: An Ultrafast FRET Study", J. Phys. Chem. B, 116 (2012) 7841.
3. S. Banerjee, D. Bhowmik, P. K. Verma, R. K. Mitra, A. Siddhanto, G. Basu and S. K. Pal "Ultrafast Spectroscopic Study on Caffeine Mediated Dissociation of Mutagenic Ethidium from Synthetic DNA and Various Cell Nuclei", J. Phys. Chem. B 115 (2011) 14776.
4. S. Banerjee and S. K. Pal "Caffeine Mediated Dissociation of a Potential Mutagen from DNA Mimetics, DNA and Cellular Nuclei: Ultrafast Spectroscopic Studies", Int. Review of Biophysical Chemistry, 3 (2012) 173.
5. S. Banerjee, S. Sarkar, K. Lakshman, J. Dutta and S. K. Pal "UVA Radiation Induced Ultrafast Electron Transfer from a Food Carcinogen Benzo[a]Pyrene to Organic Molecules, Biological

Macromolecules and Inorganic Nano Structures", J. Phys. Chem. B, 117 (2013) 3726.

6. S. Banerjee, N. Goswami and S. K. Pal "A Potential Carcinogenic Pyrene Derivative under FRET to Various Energy Acceptors in Nanoscopic Environments", ChemPhysChem, 14 (2013) 3581.
7. S. Banerjee, S. Chaudhuri and S. K. Pal "Ultrafast Spectroscopic Studies on the Interaction of a Potential Food Carcinogen with Biologically Relevant Macromolecules", Int. Review of Biophysical Chemistry, (2013)
8. T. Mondol, S. Banerjee, S. Batabyal and S. K. Pal "Study of Biomolecular Recognition Using Time-resolved Optical Spectroscopy", Int. Review of Biophysical Chemistry, 2 (2011) 211.

"Spectroscopic Investigation on Fluorescent Probes in Biologically Relevant and Engineered Environments"

Subrata Batabyal

Supervisor: Professor Samir Kumar Pal, Department of Chemical, Biological & Macro-Molecular Sciences

The use of fluorescent probes in biophysical research has been a common practice in recent years, and their use is continually increasing due to their versatility, sensitivity, quantitative capabilities, and technological applicability. Among their myriad of uses, fluorescent probes are employed to perceive biomolecular interaction, catalysis reaction, structural/conformational changes and to monitor biological processes in vivo and in vitro. From the technological viewpoint, fluorescent probes also possess immense potentials. The effect of confined engineered environments on various fluorescent probes opens up the door to investigate and interpret a broad range of problems ranging from physics to biology. Confined engineered environment results in the significant modification of the fluoroprobe properties (fluorescence intensity, emission wavelength, fluorescence lifetime etc.) due to the geometrical restriction and interactions with the confining framework, thus providing important information about the system under study. The key focus of this thesis is to explore the detail spectroscopic properties of various kinds of fluoroprobe including organic dyes/drugs and inorganic semiconductor QDs in different host environments of biological and technological interest. Many key chemical and biochemical reactions, particularly in living cells, take place in confined space at the microscopic scale. While exploring the biological/biomimetic cavities and interface, we investigated the solvent relaxation of acrylodan probe residing in the cleft of Serum albumin and inside a reverse micelle. Förster resonance energy transfer (FRET) was employed to monitor the distance between donor (tryptophan) and acceptor (acrylodan) and hence the dynamical and structural fluctuation over the time and over a wide temperature range. We also explored the interfacial water dynamics and DNA side chain flexibility using Hoechst 33258 (H258), a well-known DNA minor groove binder, in specific protein-DNA interaction between lambda repressor protein and different operator DNA. The effect on the exchangeability of minor groove water molecules with the bulk water molecules in protein-DNA complex was investigated using temperature dependent solvation study on H258. To capture and analyze the intermediate state of molecular recognition, an optofluidics platform was indigenously developed by coupling microfluidics to fluorescence spectrophotometer and fluorescence microscopy. Molecular recognition of small molecules (drugs/ligands) with biomimetic and biological macromolecules was studied in the confined microchannel by collecting fluorescence image and lifetime along the microchannel at well-defined

positions. The platform also demonstrated the capability of monitoring fast reaction kinetics of a model ionic reaction. The technologically relevant engineered environments and its effect on the emission properties of closely placed emitter (QDs) was also studied. In this respect, the effect of optical interference created by silver/silicon reflective surface on QDs fluorescence was systematically investigated. CdSe/ZnS QDs and QDs-merocyanine conjugate were placed in front of reflective silver/silicon surface at different distance by poly vinyl alcohol (PVA) spacer layers of different thickness to monitor the effect of optical interference on their excited state lifetime and its implication in biological arena (quantum yield calculation of intrinsic fluorophore) and in technological perspective (OLED, QDs based solar cell). In this direction, a quantitative and mechanistic study on excited state fluorescence lifetime of QDs on contact mode of silver film was carried out in order to understand the photon-plasmon interaction phenomenon.

List of publications:

1. S. Batabyal, T. Mondol and S.K. Pal, Picosecond-resolved solvent reorganization and energy transfer in biological and model cavities. *Biochimie*, 95 (2013) 1127.
2. S. Batabyal, T. Mondol, S. Choudhury, A. Mazumder and S.K. Pal, Ultrafast interfacial solvation dynamics in specific protein DNA recognition. *Biochimie*, 95 (2013) 2168.
3. S. Batabyal, S. Rakshit, S. Kar and S.K. Pal, An improved microfluidics approach for monitoring real-time interaction profiles of ultrafast molecular recognition. *Rev. Sci. Instrum.*, 83 (2012) 043113.
4. S. Batabyal, T. Mondol, K. Das and S.K. Pal, Förster resonance energy transfer in a nanoscopic system on a dielectric interface. *Nanotechnology*, 23 (2012) 495402.
5. S. Batabyal, A. Makhal, K. Das, A.K. Raychaudhuri and S.K. Pal, Ultrafast dynamics of excitons in semiconductor quantum dots on a plasmonically active nano-structured silver film. *Nanotechnology*, 22 (2011) 195704.
6. S. Batabyal, S. Choudhury, D. Sao, T. Mondol and S.K. Pal, Dynamical perspective of protein DNA interaction. *Biomol Concepts*, In Press (2014).
7. T. Mondol, S. Batabyal and S.K. Pal, Interaction of an antituberculosis drug with nano-sized cationic micelle: Förster resonance energy transfer from dansyl to rifampicin in the microenvironment. *Photochem. Photobiol.*, 88 (2012) 328.
8. T. Mondol, S. Batabyal, A. Mazumder, S. Roy and S.K. Pal, Recognition of different DNA sequences by a DNA-binding protein alters protein dynamics differentially. *FEBS Lett.*, 586 (2012) 258.
9. T. Mondol, S. Batabyal and S.K. Pal, Ultrafast electron transfer in the recognition of different DNA sequences by a DNA-binding protein with different dynamical conformations. *J. Biomol. Struct. Dyn.*, 30 (2012) 362.
10. S. Chowdhury, S. Batabyal, D. Sao, T. Mondol and S.K. Pal, Ultrafast dynamics of solvation and charge transfer in a DNA-based biomaterial. *Chem. Asian J.*, DOI: 10.1002/asia.201400062 (2014).
11. T. Mondol, S. Banerjee, S. Batabyal and S.K. Pal, Study of biomolecular recognition using time-resolved optical spectroscopy. *Int. Review of Biophysical Chemistry*, 2 (2011) 211.

STUDENTS' PAGE

लकीरें
(राज कुमार साधु)

लकीरें तो पहले भी था, अब भी है, उन्हें रहने दो
जुबां से अपनी चीख चीख कर, इतिहास उन्हें कुछ कहने दो
कभी कोई यँही खिंच दिया था, इंसान या शैतानो ने
या अपने किसी स्वार्थ के खातिर, अपने या बेगानो ने
मिटाने से अब मिटेगा ना ये, दाग बहुत ही गहरा है
खिलते थे जहाँ फूल खुशी के, अब तो गम का पहरा है
चलो बनाकर पाला इनको, मिलकर कबड़ड़ी खेले हम
खो जायेगा बैर सारा, मिट जायेगा सारा गम
बाँट लो अपनी खुसिया सब से, गम भी सबको सहने दो
लकीरें तो पहले भी था, अब भी है, उन्हें रहने दो

कुछ लकीरें बसा है तन में, कुछ है अपने मन में बुना
कुछ है अपने यादों में और कुछ दूसरों से सुना सुना
कुछ को तो हमने ही पाला, ऊँच-नीच और भेद बढ़ाया
कुछ को तो यूँ सींच-सींच कर इतना बड़ा बनाया
मिटाने से अब मिटेगा ना ये, दाग बहुत ही गहरा है
खिलते थे जहाँ फूल खुशी के, अब तो गम का पहरा है
बना के उनको लक्ष्मण रेखा, रक्षा करो हर सीता की
हर रावण को रोको बाहर, लाज रखो हर माता की
द्वेष घृणा और अंधेपन को आँसू बनकर बहने दो
लकीरें तो पहले भी था, अब भी है, उन्हें रहने दो

1st Inter-Institute Badminton Tournament-2014

*Organised by the Sports Activity Group of
MUKTANGAN, SNBNCBS*

It was 22nd February 2014. It was a very soothing and sunny winter day. It was not like usual weekend day for the students and staffs of SNBNCBS. Each and every person of SNBNCBS was quite excited and feeling proud for being a part of the SNBNCBS family, which is going to organize the 1st Inter-Institute Badminton Tournament-2014 with the help of the sports activity group of MUKTANGAN, SNBNCBS at SNB badminton court arena. All the arrangements were done in a very well organized fashion for organizing this badminton tournament named "Battle of Smashes". This tournament was result of the hard work of Debasish Das Mahanta, a die-hard fan of badminton, who sketched the outline of this tournament with his volunteers team, as well as the court curators (Mr. Nitai Saha and Mr. Nilmoni Jana's team) who gave their full will power to make this tournament a great success. Every spectator's wait came to an end when the tournament was inaugurated by our respected Director Prof. Arup Kumar Raychaudhuri along with Registrar Ms. Shohini Majumder.

The whole tournament was split into three formats: "Men's Doubles", "Woman's Singles", and "Mixed Doubles". In each format, 16 teams participated from different institution viz. S.N. Bose National centre for Basic Sciences (SNBNCBS), Indian Institute of Chemical Biology (IICB), Bose Institute, Netaji Subhash Engineering College (NSEC), Future Institute of Engineering and Management (FIEM), Saha Institute of nuclear Physics (SINP), Indian Association of Cultivation of Sciences (IACS), Variable Energy Cyclotron Centre (VECC) from outside participated in the tournament. After one day of league matches among the teams on 23rd February 2014, the final matches took place. In Men's Doubles format the final match took place between two unbeatable teams (Debasish Das Mahanta & Samiran Choudhary) SNBNCBS vs (Muruganandan Thangamuniyandi & Sapan Mandloi) IICB. In the high voltage match at the packed arena, again it was a nail biting finish ending in the final game and the IICB team put their best to overcome the host team and became the champion of the 1st Inter-Institute Badminton Tournament-2014.

More interestingly, in Woman's Singles format host institution girls were unbeatable. In the final, Shaili Sett (SNBNCBS) beat her opponent Semanti Pal (SNBNCBS) in a very challenging match and secured the champion's trophy for the host institute. Surprisingly, in the Mixed Doubles format, (Sreeraj TP and Chaoba Yendrembam) SNBNCBS defeated many favourite teams of the spectators and set their final match with unstoppable (Thangamuniyandi and Sayani Bannerjee) IICB. In the final match, IICB held their nerves to clinch it by the small margin and became the champion. All the players from different institutes showed good sportsman spirit throughout the tournament. At the end, all the participants received T-shirt designed by MUKTANGAN, with (Champions) 1st, 2nd & 3rd place competitors receiving their magnificent trophies and certificates. The organizers offered their sincere thanks to all the participating institutes. In return, participant of different institution were very thankful to the organizers for their hospitality. In future, they are very much interested to organize such kind of events in collaboration with us.



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