

National Level Academic Review

A Report for the period 2012-2017

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- **BIOPHYSICS & STRUCTURAL GENOMICS
(B&SG) DIVISION**
 - **CRYSTALLOGRAPHY & MOLECULAR BIOLOGY
(C&MB) DIVISION**
 - **CHEMICAL SCIENCES DIVISION (CSD)**
 - **COMPUTATIONAL SCIENCE DIVISION**

National Level Academic Review

Biophysics & Structural Genomics Division (B&SG)

A Report for the period 2012-2017

Divisional Staff	
Scientific/Engineer	Technician/Scientific Assistants
Subrata Banerjee, Professor -'H'	Ajay Chakarabarti (EMF)
Debashis Mukhopadhyay, Professor-'G'	Arijit Pal
Oishee Chakrabarti, Assoc. Professor-'F'	Nirmal Das
Kaushik Sengupta, Assoc. Professor-'F'	Raju Dutta
Chandrima Das, Assoc. Professor-'E'	M. Mahendra (EMF)
Sangram Bagh, Assoc. Professor-'E'	
Soumen Manna, Assoc. Professor-'E'	
	Scientific Officer
Pulak Ray, Engineer -'G' & Head, Electron Microscope Facility (EMF)	Mr. Shekar Bhattacharjee <i>(Deceased)</i>
	Administrative/Auxiliary
Faculty Superannuated	Mahuya Dutta
Prof. Pradeep K. Sengupta, 2012	Shyamal Digar
Prof. Arun K. Pal, 2013	Sanjoy Shaw
Prof. Dipak Dasgupta, 2015	Madhusudan Shyamal

Postdoctoral Fellows (PDF):		
No.	Name (Supervisor)	Year of joining
1.	Dr. Shravanti Mukherjee (<i>Prof. Chandrima Das</i>)	2016
2	Dr. Siddhi Chaudhuri (<i>Prof. Debashis Mukhopadhyay</i>)	2017
3	Dr. Biswadeep Chaudhuri (<i>Resigned, July 2017</i>)	2016

Project Assistants (PA):		
No.	Name (Supervisor)	Year of joining
1.	Sulagna Sanyal (<i>Prof. Chandrima Das</i>)	2015
2	Subarna Dutta (<i>Prof. Kaushik Sengupta</i>)	2015
3.	Souvik Ghosh (<i>Prof. Chandrima Das</i>) <i>Resigned July 2017</i>	2016

Research Fellows (RFs)			
No.	Name	Year of joining	Ph.D. Supervisor
1	Piyali Majumdar	2012	Prof. Debashis Mukhopadhyay
2	Zenia Kaul	2012	Prof. Oishee Chakrabarti
3	Sayasachi Sen	2012	Prof. Chandrima Das
4	Isha Sengupta	2012	Prof. Chandrima Das
5	Debdattoo Mookerjee	2013	Prof. Oishee Chakrabarti
6	Saran Chattopadhyay	2014	Prof. Subrata Banerjee
7	Sudeshna Pal	2014	Prof. Soumen Manna
8	Sayak Mukhopadhyay	2015	Prof. Sangram Bagh
9	Kathakali Sarkar	2015	Prof. Sangram Bagh
10	Tanushree Chakraborty	2015	Prof. Soumen Manna
11	Rajdeep Das	2015	Prof. Oishee Chakrabarti
12	Payal Mondal	2015	Prof. Chandrima Das
13	Suparna Saha	2015	Prof. Debashis Mukhopadhyay
14	Kaushik Chanda	2015	Prof. Debashis Mukhopadhyay
15	Sweta Singh	2015	Prof. Subrata Banerjee

Ph.D. Thesis Submitted:				
No.	Name	Supervisor	Year	Current Position
1.	Rukmini Mukherjee	Prof. Oishee Chakrabarti	2016	Postdoc, UCLA, USA
2.	Manindra Bera	Prof. Kaushik Sengupta	2016	Postdoc, Rockefeller U., USA
3.	Sudha Bucha	Prof. Debashis Mukhopadhyay (<i>Co-Supervisor</i> : Prof. N.P. Bhattacharyya)	2017	

Ph.D. degree Awarded (2012 - todote)				
No	Name	Supervisor	Award	Present Status
1	Sutapa Saha	Abhijit Chakrabarti	2012	Faculty, Presidency Univ., Kolkata
2	Sibojyoti Lahiri	Dipak Dasgupta	2012	Postdoc, Ludwig- Maxmillians, Univ. Munich, Germany
3	Parijat Majumdar	Dipak Dasgupta	2013	Postdoc, Max Planck Inst. of Biochemistry, Germany
4.	Aditi Sengupta Banerjee	Subrata Banerjee	2013	Res. Assoc., NCI, NIH, Bethesda, MD, USA
5	Samir Das	Debashis Mukhopadhyay (<i>Co-Supervisor: Uday Sen</i>)	2013	Postdoc, Univ. British Columbia, Canada
6	Biswapathik Pahari	Pradeep K. Sengupta	2013	
7	Sudipta Pal	Dipak Dasgupta	2013	
8	Anita Roy	Subrata Banerjee	2014	Postdoc, Ludwig Inst. Of Can. Res., Belgium
9	Arunabha Chakrabarti	Debashis Mukhopadhyay	2014	DBT-Welcome Early Career Fellow, Tata Cancer Translational Centre, Kolkata
10	Saptarni Ghosh	Dipak Dasgupta	2014	Boston Univ., USA
11	Kasturi Roy	Debashis Mukhopadhyay	2014	Postdoc., Yale Univ., CT, USA
12	Amrita Banerjee	Dipak Dasgupta	2015	Postdoc, CSIR-IICB, Kolkata
13	Shreyasi Dutta	Dipak Dasgupta	2015	Postdoc, SN Bose Centre, Kolkata
14	Anindita Deb Pal	Subrata Banerjee	2015	Faculty, GD Birla College, Kolkata
15	Nandini Pal Basak	Subrata Banerjee	2015	Postdoc, NCBS, Bengaluru
16	Suchismita Halder	Abhijit Chakrabarti	2015	Postdoc., U. Kentucky, USA
17	Avik Basu	Abhijit Chakrabarti	2015	Postdoc. U. Toronto, Canada
18	Shilpita Karmakar	Abhijit Chakrabarti	2015	Postdoc., CWRU, Cleveland, OH, USA
19	Saunak Bakshi	Debashis Mukhopadhyay	2015	Postdoc., CWRU, Cleveland, OH, USA
20	Mohor Biplab Sengupta	Debashis Mukhopadhyay	2016	Postdoc., NEI, NIH, Bethesda, MD, USA
21	Srijan Halder	Subrata Banerjee	2016	Assoc. Res. Sc., Integral Biosciences, NOIDA
22	Pritha Bhattacharjee	Kaushik Sengupta	2016	CNRS, France
23	Avinanda Banerjee	Kaushik Sengupta	2016	NCBS, Bangalore
24	Devika Srivastava	Oishee Chakrabarti	2017	Postdoc, Mt. Sinai School of Med., NY, USA
25	Priyanka Majumdar	Oishee Chakrabarti	2017	Postdoc, NII, Delhi
26	Madhurima Mitra	Abhijit Chakrabarti	2016	DBT Postdoc, CSIR-IGIB, Delhi;
27	Debasree Das	Abhijit Chakrabarti	2017	SERB Postdoc, Univ. of Hyd.

Important equipments and facility

Cell Culture

- Class II Biosafety Cabinet;
- Carbon Dioxide Incubator;
- Microgravity Chamber & Hypoxic incubator;
- Flow Cytometry Cell Sorter and Analyzer (*FACS-Aria, Caliber*);

Proteomics, Lipidomics & Mass Spectrometry

- 2D-DIGE facility;
- MALDI TOF-TOF MS MS;
- ESI Q-TOF MS;
- GC-MS;

Biophysical Characterization

- Dynamic Light scattering Setup (DLS);
- Circular Dichroism (CD) and Fluorescence Spectroscopy Setup;
- Isothermal Calorimetry (ITC);
- Differential Scanning Calorimeter (DSC);

Imaging

- Super resolution Microscopy;
- Multiphoton Setup - FRAP, FLIM, FCS;
- Laser Microdissection setup;
- 200keV TEM (EMF);

Research

Saha Institute of Nuclear Physics has been working in different branches of theoretical and experimental disciplines of biophysical sciences since the early fifties. Under the inspiration and active support of the visionary Prof. Meghnad Saha, one of the oldest schools of Biophysics in India was formed. An electron microscope, the first of its kind in Asia, was fabricated indigenously in the institute under the able stewardship of Prof. N. N. Dasgupta. Since then, pioneering work was done on microscopic characterization of infectious microorganisms, cellular architectures and Radiation Biology. Subsequently, research in various fields of

Structural Biology and Spectroscopy was initiated to understand the interactions of the biologically important molecules. In the post genomic era, the immense potential of the area where physics meets biology, led to the formation of a new division- “Biophysics & Structural Genomics” in 2013. Our scientists are now actively involved in interdisciplinary area of basic and clinical research - Proteomics, Biomolecular Recognition: Chemical and Structural Biology, 'in silico' and synthetic biology. Some of the important research highlights in the area:

- **Chromatin Biology & Epigenetics:**

Mammalian genome is organized into a highly ordered nucleoprotein complex known as chromatin. Several small modifications both in DNA and protein component of chromatin fine-tune the underlying gene expression programs, genome repair as well as replication and are coined as epigenetic modifications. The molecular mechanism of epigenetic modification based functions is operated through the protein which recognizes this modification and thereby differentially recruits several other regulatory factors. The research focus of our laboratory is to understand some of these *epigenetic readers* in the context of cellular functions and their possible connection to the disease, including metabolic as well as infectious diseases. The broad areas of research include:

(a) Chromatin modifications in cancer manifestation: Cancer metastasis is still a major threat, where enhanced migratory potential and invasiveness of cancer cells, attribute it to be clinically challenging. These phenotypes are achieved by precise alteration of metastasis-associated genes through local epigenetic modifications which are recognized by a class of proteins termed as *chromatin reader* (*J Biol. Chem.*, 2016, 291, 2664; *Biochem J*, 2017, 474, 1919; *Biochim Biophys Acta*, 2017, 1860, 450).

(b) Epigenetic regulation of chromatin through heterochromatinization: Signal dependent ordered compaction of genome is guided by different histone modifications and several chromatin interacting nonhistone proteins (like HP1 α , PARP1, PC4 etc). We are in the process of identifying several cellular enzymes that can interact with chromatin activating/silencing complex thereby regulating transcription (*J Biol. Chem.*, 2015, 290, 20893).

(c) Regulation of host-response pathways by multi-functional transcription factors to during HBV pathogenesis: Research of our laboratory is also aimed to harness the scope of epigenetic therapy to Hepatitis B virus clearance. Interestingly, we have observed that viral oncoprotein HBx hijacks *chromatin reader* proteins resident in PML-NBs thereby regulating the immune response pathways to promote HBV proliferation. Thus, targeting these host transcription factors could have potential to combat HBV pathogenesis.

(d) Metabolic alteration and the transcription regulation: the epigenetic interface: Recognition of the dynamic epigenetic signatures by *chromatin readers* under nutritional stress

in metabolically active tissues (like hepatocytes) and subsequently in diabetes patients is another research focus of our laboratory. Such *reader* proteins are critical in aiding the cells to cope-up with the changing glycemic environment by influencing metabolic gene expression, and act like glucose sensors for metabolically active tissues.

(e) Therapeutically important small molecules as regulators of epigenetic modifications: Besides understanding the chromatin modification based genome dynamics of the *chromatin readers*, the functions of several therapeutically important small molecules, which has potential to reprogram the epigenetic landscape of chromatin and consequent gene expression programs, are being investigated in collaboration with several chemical biologist groups (*Biochim Biophys Acta*, 2017, 4165,30131; *Biochem. Biophys. Res. Commun.* 2015, 462,352; *FEBS Open Bio.* 2014, 4, 987).

- **Deciphering the Molecular Players in Neuro Re-/De-generation**

The primary goal of human neurodegenerative disease (NDD) research over the last decade had been deciphering of the underpinning molecular mechanisms, especially in the case of complex Alzheimer's (AD) and Huntington's (HD) diseases. The emerging model was later extended to other modalities like regenerating Spinal Cord Injury (SCI) and demyelinating Neuromyelitis Optica (NMO). The common theme across this disorder spectrum had been their progressive and fatal nature, commonly characterized by the intracellular or extracellular presence of abnormal protein aggregates.

Comparison of the crystal structures of APP Intracellular Domain (AICD) peptides bound to its adapter Grb2 revealed a conformational switching of AICD and it was proposed that its natively unfolded regions gain specific conformation after association with interacting partners. Twenty novel potential interacting partners for unphosphorylated AICD were identified by *in vitro* pull-down experiments followed by 2D gel electrophoresis and MALDI-MS. The cellular functions of several of these novel interactors can be correlated with AD and might further elucidate AICD's involvement in disease pathogenesis. During this period the group has demonstrated the interaction of the adapter Grb2, otherwise a growth related protein, with other proteins having roles in neurodegenerative conditions, probably to save the neurons from the cytotoxic load. The compartments formed due to the Grb2 overexpression (a situation mimicking the NDD conditions) were identified as autophagosomes. Grb2 mediated aggregation prevention of Huntingtin (Htt) and its autophagic clearance has also been investigated.

Complimentary to the program above it was realized that Neuro-regeneration could just be a process played by similar players in a different biological context. Spinal cord injury (SCI) was chosen as a model to study this process. 2-Dimensional difference gel electrophoresis (2D-DiGE)

was used to examine the differential expression of the human CSF proteome from different SCI categories ranging from most severe to least severe. The analysis yielded 8 candidate proteins with differential expression and possible implications in the post-SCI phenotypes.

- **Nuclear lamins: Important regulators of nuclear architecture and homeostasis**

Nuclear Lamins form a 10 nm thick meshwork underlying the inner nuclear envelope of all eukaryotic cells. These laminar structure help in the tethering of chromosome at the nuclear periphery as well as the proper positioning of the nuclear pore complex. Lamins also play vital roles in transcription, replication and DNA damage response. More than 450 mutations have been uncovered in A-type lamins which lead to a plethora of diseases termed as laminopathies. Laminopathies include mainly different types of muscular dystrophies, lipodystrophies and premature aging syndromes including multiple organ failure. My laboratory is focussed on understanding the role of mutant lamin A/C in the pathogenesis of Dilated Cardiomyopathy (DCM) - a class of muscular dystrophy. Nuclei from DCM affected patients are characterized by misshapen and fragile nuclei with reduced elasticity. We have shown the structural alteration of some of the mutants of lamin A which produce severe phenotypes in patients. Alongside we established that the viscoelasticity of the lamina is altered in the case of lamin A mutants. We used a variety of methods for elucidating this at the bulk level as well as single molecule level. It logically follows that the nuclear envelope which is supported by the laminar framework gets eventually weakened and distorted and succumbs to the disease phenotypes. We also followed up a clinical study with patients suffering from idiopathic DCM and identified 8 novel SNPs associated with the disease. Currently we have been extending our understanding of nuclear and cellular elasticity in matrix based cardiac tissue differentiation in the light of lamin A mutations. On a different note we are also investigating the role of lamin proteins in DNA damage response mechanisms on cancer models.

- **Organellar biogenesis and dysfunction during late onset-neurodegeneration:**

From a socio-economic point of view, neuropathies are on the rise globally and also in India since the average age of the population and its longevity are progressively increasing. Even in this day and age, afflicted individuals are marginalised and any discussion about them is a taboo. Hence multidimensional basic research, as highlighted in this study is an absolute necessity for better therapeutics to alleviate the pain, suffering and associated social stigma. The mechanisms leading to disease are not fully understood, but it is plausible to hypothesize that in addition to the gain of new toxic properties of protein aggregates, loss of wild-type function of interacting proteins also contributes to pathogenesis. During the past five years we

have extensively used confocal microscopy based imaging on fixed as well as live cells to follow various cellular phenomena, like assembly of mitotic spindles, cell division, microtubule regrowth (*Cell Death and Disease*, 2014; *Biochemistry and Cell Biology*, 2015, 2016), vesicular fusion between late endosomes and lysosomes, endocytic trafficking (*Cell Death and Disease*, 2015; *Biochemistry and Cell Biology*, 2016; *Molecular Neurobiology*, 2017), internalisation of mitochondria inside autophagosomes leading to mitophagy, tracked movement of mitochondria inside neuronal processes (by retinoic acid treatment of SHSY5Y cells), followed fission and fusion of mitochondria, cell fusion assays (*Journal of Cell Science*, 2016; *BBA - Molecular Cell Research*, 2016), studied ER stress mediated apoptosis (*Molecular Biology of the Cell*, 2017). While trying to understand the cell biological events leading to neurodegeneration, my laboratory has made multiple significant contributions in general. We have established that (i) tubulin ubiquitination is a factor in determining left-right symmetry of the body, (ii) ESCRT proteins affect fusion between late endosomes and lysosomes, (iii) trans ubiquitination of ER E3 ligase by cytosolic E3 ligase regulates mitophagy, (iv) identified the sequence of events that lead to mitochondrial fusion in mammals, (v) involvement of ESCRT proteins in ER stress mediated apoptosis. Currently we are extending this to understand how ERAD tuning is instrumental in regulating mitochondrial dynamics – compromised response to ER stress and altered mitochondrial fission-fusion dynamics being two key factors in most late-onset neurodegenerative diseases.

- **Synthetic and Systems Biology**

We have started our synthetic biology lab little more than two years back with the goal to create a synthetic biology platform for performing complex cellular computation and its application in programmed delivery of therapeutic bio-molecules in cancer cells and in space bioengineering. We have recently established a systems biology pipeline and analyze the effect of microgravity on global gene expression data of human (*Scientific Reports 2016*) and bacterial cells (*Astrobiology 2016*) from space and simulated microgravity experiments. We have found multiple new pathways, network and new insight, which were not possible by conventional analysis. This study indicates some new disease signatures in microgravity, including few types of cancers, may help assessing risks of long duration space travel and developing new space medicine. The works also suggest plausible molecular reasoning for previously unexplained facts related to space travel including the altered smelling behaviour of astronauts, the increased survival of salmonella in macrophages in microgravity and deregulation upstream signalling pathways in immunity. On the other hand, we are forward engineering artificial computation/intelligence in living cells using complex synthetic gene circuits. In that direction, currently we are building an electronic analogous genetic decoder in living bacterial cells for decoding extracellular chemical signals in digital fashion. Further we have created a synthetic

genetic device, which can tune the vertical scaling factor for genetic signal response curve predictively. We have also created a biobrick type plasmid vector for easy integration of multiple genetic cascades in any direction with the help of only four restriction enzymes.

- **Lipidomics & Metabolomics**

Non-alcoholic fatty liver disease (NAFLD): Apart from its asymptomatic nature, lack of understanding of NAFLD pathogenesis and progression renders preventive or curative intervention challenging. We are examining the metabolic reprogramming associated with lipid accumulation in hepatocytes and the contribution of chronic malnutrition on initiation and progression of NAFLD using cell lines. Cell line-based model for composite alcoholic and non-alcoholic steatosis is being developed to delineate signatures representing mixed aetiology. MALDI-MS based imaging protocol has been developed in-house that will eventually be used for differential diagnosis of alcoholic and non-alcoholic fatty liver disease through tissue imaging.

Sub-cellular metabolic reprogramming in cancer: Abnormal behaviour of cell is essentially a reflection of the aberration in the function sub-cellular compartments. Loss of this spatially resolved information on cellular biochemistry in whole cell-based metabolic and proteomic experiments may be the reason behind our inability to understand the heterogeneity in disease progression and therapeutic response in cancer. We have established protocols for isolation of nucleus and extraction of metabolites thereof. Currently standardization of protocol for isolation of mitochondria and endoplasmic reticulum is ongoing. We will eventually examine the nature of proteo-metabolomic changes at different cellular compartments upon exposure to oxidative and nutritional stress and their role in determining cell fate. Role of RNA methylation in reorganization of the biochemical landscape during stress response will also be investigated to rationalize the heterogeneity in behaviour of cancer cells.

FUTURE PLANS: *From architectural and metabolic reorganization in cancer cells to development of novel therapeutic strategies*

India is plagued by an estimated one million disparate cases of cancers every year with about 60 – 70% mortality rate. The number of cases is projected to shoot up to 1.73 million by 2020. Of these, a few forms of cancer show selective preponderance in India as opposed to the rest of the world and entice our interest. Triple Negative Breast Cancer (TNBC), with poor prognosis

due to the high frequency of early relapse and metastasis, has an overall prevalence of about 31% of the 0.15 million new cases of Breast Cancer per year. Gynaecological cancers of the cervix, ovary, rectum and colon form the next tier of cases in the Indian scenario. Hepatobiliary malignancies, particularly gallbladder cancer, one of the deadliest forms of cancer with mean survival period of 6 months from diagnosis, 5-year survival rate of <10% and high rate of relapse even after surgical resection and treatment, shows an abnormally high incidence among north and north-east populations. Tumours of the central nervous system (CNS) constitute 1–2% of all malignancies world-wide. In India, an alarming increase (almost double) in incidences of tumours of the CNS has been recorded with less than 3% survival beyond 3 years.

So far there is a rich literature to support that intra- and extra-cellular signalling pathways are perturbed during the genesis of cancer. Similarly, there are abundant evidence to support that alterations in cell cycle check points destabilize a “normal” cell towards a “cancerous” fate. Cancer signalling pathways have become the central research theme for developing chemotherapeutic, biologic and RNA-based targeted therapy. On the other hand, emerging evidence suggests a consonance of dynamic changes in intracellular architecture, epigenetic modifications and metabolic reprogramming with cancer, which can be targeted for developing a novel therapy. However, this area is explored poorly worldwide. To our knowledge, no major effort has been put in India to look at cancers beyond signalling pathways. It is also not known how tumor-microenvironment interactions influence the metabolic landscape leading to therapeutic resistance and relapse. Here we propose to elucidate and intervene with these aspects to search for novel therapeutic strategies. We have formed an interdisciplinary team with expertise in various fields including epigenetics, proteomics, metabolomics, mechanobiology, organelle biology and synthetic biology to address the following questions:-

Question I: Does reorganization of cellular architecture correlate to early detection and therapeutic intervention of cancers?

Question II: Does sub-cellular metabolic reprogramming, in connivance with tumor-microenvironment interaction, dictate the ability of cancer cells to thrive under radiation, redox and xenobiotic stress?

List of Publication (2012-2017)

(Total No. =119)

2017

1. Basu M *et al.*, Dual histone reader ZMYND8 inhibits cancer cell invasion by positively regulating epithelial genes. *Biochem J.* 2017; 474(11): 1919-1934.
2. Basu M *et al.*, Chromatin reader ZMYND8 is a key target of all trans retinoic acid-mediated inhibition of cancer cell proliferation. *Biochim Biophys Acta- Gene Regulatory Mechanisms.* 2017; 1860(4): 450-459.
3. Das D, *et al.*, Anti-hepatitis B virus (HBV) response of imiquimod based toll like receptor 7 ligand in HBV - positive human hepatocellular carcinoma cell line. *BMC Infect Dis.* 2017; 17(1): 76.
4. Goswami S *et al.*, Interaction of a Common Painkiller Piroxicam and Copper-piroxicam with Chromatin Causes Structural Alterations Accompanied by Modulation at the Epigenomic/Genomic level. *Biochim Biophys Acta- General Subjects.* 2017; 4165(17): 30131-9.
5. Majumder P *et al.*, Cellular levels of growth factor receptor bound protein 2 (Grb2) and cytoskeleton stability are correlated in a neurodegenerative scenario. *Dis Model Mech.* 2017 Mar 30.
6. Sengupta MB *et al.*, Increased expression of ApoA1 after neuronal injury may be beneficial for healing. *Mol Cell Biochem.* 2017; 424(1-2): 45-55.
7. Banerjee A *et al.*, The plant alkaloid chelerythrine binds to chromatin, alters H3K9Ac and modulates global gene expression. *J. Biomol. Struct. Dyn.* 2017; 35(7): 1491-1499
8. Dey SK *et al.*, Differential role of nonmuscle myosin II isoforms during blebbing of MCF-7 cells. *Mol Biol Cell.* 2017;. pii: mbc.E16-07-0524. doi: 10.1091/mbc.E16-07-0524. [Epub ahead of print]
9. Kaul Z and Chakrabarti O. Tumor susceptibility gene 101, TSG101, regulates predisposition towards apoptosis via ESCRT machinery accessory proteins. *Mol Biol Cell*, 2017; epub ahead of print, doi: 10.1091/mbc.E16-12-0855
10. Majumder P and Chakrabarti O. Lysosomal quality control in Prion diseases. *Mol Neurobiology*, 2017; epub ahead of print, doi: 10.1007/s12035-017-0512-8
11. Mukherjee R *et al.*, Calcium dependent regulation of protein ubiquitination – interplay between E3 ligases and calcium binding proteins. *Biochim Biophys Acta - Molecular Cell Research*, 2017; 1864: 1227-1235
12. Patel D *et al.*, Unique and Novel Urinary Metabolomic Features in Malignant versus Benign Adrenal Neoplasms. *Clin. Cancer Res.* 2017; PMID: 28450405

2016

1. Adhikary S *et al.* Selective Recognition of H3.1K36 dimethylation / H4K16 acetylation facilitates the regulation of ATRA-responsive genes by putative chromatin reader ZMYND8. *J Biol Chem.* 2016; 291: 2664-81.
2. Das D. *et al.* Anti-viral role of toll like receptor 4 in hepatitis B virus infection: An *in vitro* study. *World J Gastroenterol.* 2016; 22(47):10341-10352.
3. Bandopadhyay M *et al.* Hepatitis B virus X protein mediated suppression of miRNA-122 expression enhances hepatoblastoma cell proliferation through cyclin G1-p53 axis. *Infect Agent Cancer.* 2016; 11:40

4. Banerjee A *et al.* The plant alkaloid chelerythrine binds to chromatin, alters H3K9Ac and modulates global gene expression. *J Biomol. Struct. Dyn.* 2016; 5: 1-9.
5. Sengupta MB, Mukhopadhyay D. Possible role of apolipoprotein A1 in healing and cell death after neuronal injury. *Front Biosci (Elite Ed)*. 2016; 8: 460-77.
6. Baksi S. *et al.* Systemic study of a natural feedback loop in Huntington's disease at the onset of neurodegeneration. *Biosystems*. 2016; 150: 46-51.
7. Sengupta MB. *et al.* Clinical proteomics of enervated neurons. *Clin Proteomics*. 2016; 13: 10.
8. K Roy Chowdhury *et al.* Chaperone-like protein HYPK and its interacting partners augment autophagy., *Eur. J. of Cell Biol.*, 2016; 95(6-7):182-94.
9. Chakraborty SD *et al.* Development of a Triplet-Triplet Absorption Ruler: DNA- and Chromatin-Mediated Drug Molecule Release from a Nanosurface. *J Phys Chem B* .2016; 120(27):6872-81.
10. Maity S. *et al.*, Inhibition of Porcine Pancreatic Amylase Activity by Sulfamethoxazole: Structural and Functional Aspect. *Protein J*. 2016; 35(3):237-46.
11. Karthigeyan D. *et al.* A Dual Non-ATP Analogue Inhibitor of Aurora Kinases A and B, Derived from Resorcinol with a Mixed Mode of Inhibition. *Chem Biol Drug Des*. 2016; 87(6):958-67
12. Mukherjee M and Chakrabarti O. Regulation of Mitofusin1 by Mahogunin Ring Finger-1 and the proteasome modulates mitochondrial fusion. *Biochimica et Biophysica Acta (BBA) - Molecular Cell Research*, 2016; 1863:3065-3083
13. Bera K *et al.* Metamorphosis of Ruthenium Doped Carbon Dots: In Search for Origin of Photoluminescence and Beyond. *Chem. of Mat.*, 201; 28: 7404–7413
14. Srivastava D. *et al.* Mahogunin mediated regulation of G α , localisation during mitosis and its effect on spindle positioning. *Biochem. and Cell Biol.*, 201; 94, 359-69
15. Majumder P and Chakrabarti O. ESCRTs and associated proteins in lysosomal fusion with endosomes and autophagosomes. *Biochem. and Cell Biol.*, 2016;.epub ahead of print, 1-8
16. Mukherjee R and Chakrabarti O. Ubiquitin mediated regulation of the E3 ligase GP78 by Mahogunin in trans affects mitochondrial homeostasis. *J. Cell Science* 2016; .pii: jcs.176537
17. Bera M.*et al.*, Significance of 1B and 2B domains in modulating elastic properties of lamin A. *Scientific Rep.*; 2016; 6:27879
18. Dutta S *et al.*, Implications and assessment of the elastic behavior of lamins in laminopathies. *Cells* 2016; 5(4):37
19. Chakrabarti A. *et al.*, Erythrocyte & Platelet Proteomics in Haematological Disorders. *Proteomics Clin Appl*. 2016; 10: 403-414.
20. Karmakar S. *et al.*, Platelet proteomics in thalassemia. Factors responsible for hyperquagulation. *Proteomics Clin Appl*. 2016; 10: 239-247
21. Roy R. *et al.* A systems biology analysis unfolds the molecular pathways and networks of pathogenic bacteria in space flight and simulated microgravity condition, *Astrobiology*, 2016; 16: 677–689.

22. Mukhopadhyay S, *et al.* A systems biology pipeline identifies new immune and disease related molecular signatures and networks in human cells during microgravity exposure, *Scientific Rep*, 2016; 6:25975,
23. Bagh S, Reprogramming living cells with an engineering language, *Physics News*, 2016; 46: 43-52
24. Basak NP and Banerjee S. Crosstalk between Notch signaling Pathway and Glutamine uptake during Jurkat T cell activation *Matters* 2016; 2 (2), e20160200003.

2015

1. Chakrabarti R. *et al.*, Phosphatidylinositol 4-phosphate 5-kinase 1-alpha modulates ribosomal RNA gene silencing through its interaction with histone H3 lysine 9 trimethylation and heterochromatin protein HP1-alpha. *J Biol. Chem.* 2015; 290: 20893-903.
2. Banerjee A *et al.*, Recognition of chromatin by the plant alkaloid, ellipticine as a dual binder. *Biochem Biophys Res Commun.* 2015; 462:352-7.
3. Dutta S *et al.* Association of antitumor antibiotic Mithramycin with Mn²⁺ and the potential cellular targets of Mithramycin after association with Mn²⁺ .*J. Biomol. Struct. Dyn.* 2015; 33(2) 434-46
4. Lahiri S *et al.*, Association of a Zn(2+) containing metallo β -lactamase with the anticancer antibiotic mithramycin. *J Inorg. Biochem.*, 2015, 142:75-83
5. Ghosh S *et al.*, Plant alkaloid chelerythrine induced aggregation of human telomere sequence--a unique mode of association between a small molecule and a quadruplex; *Biochemistry*, 2015; 54(4):974-86
6. Ghosh S and D. Dasgupta. Quadruplex forming promoter region of c-myc oncogene as a potential target for a telomerase inhibitory plant alkaloid, chelerythrine. *Biochem Biophys Res Commun.* 2015; 459(1): 75-80
7. Roy S *et al.*, The Unfolding MD Simulations of Cyclophilin: Analyzed by Surface Contact Networks and Their Associated Metrics. *PLoS One.* 2015; 10(11):e0142173. doi: 10.1371
8. Bucha S *et al.* Regulation of mitochondrial morphology and cell cycle by microRNA-214 targeting Mitofusin2 *Biochem Biophys Res Commun.* 2015; 465(4):797-802.
9. Banerjee, A.*et al* Novel linkage of *LMNA* single nucleotide polymorphism with dilated cardiomyopathy in an Indian case study. *IJC Heart & Vasculature* 2015;99-105.
10. Roy J. *et al.*, Hsp70 clears misfolded kinases that partitioned into distinct quality-control compartments. *Mol Biol Cell.* 2015; 26(9):1583-600.
11. Bhattacharjee, P *et al.*, Molecular Events in Lamin B1 Homopolymerization: A Biophysical Characterization. *J. Phys. Chem. Part B:* 2015;119(44):14014-21
12. Majumder P and Chakrabarti O. Mahogunin regulates fusion between amphisomes/MVBs and lysosomes via ubiquitination of TSG101. *Cell Death and Disease*, 2015;.6: e1970
13. Srivastava D and Chakrabarti O. Ubiquitin in regulation of spindle apparatus and its positioning: implications in development and disease. *Biochem. and Cell Biol.* 2015; 9:, 273-281
14. Theeya N *et al.* An inducible and secreted eukaryote-like serine/threonine kinase of *Salmonella enterica* serovar Typhi promotes intracellular survival and pathogenesis. *Infection and Immunity*, 2015; 83:522-533

15. Kumari S *et al.* Identification and characterization of nonhistone chromatin proteins: human positive coactivator 4 as a candidate ***Methods Mol Biol.*** 2015; 1288:245-72.
16. Basu A and Chakrabarti A Defects in erythrocyte membrane skeletal architecture. ***Adv Exp Med Biol.*** 2015; 842:41-59
17. Karmakar S *et al.*, Differential proteomics study of platelets in asymptomatic constitutional macrothrombocytopenia: altered levels of cytoskeletal proteins. ***Eur J Haematol.*** 2015 Jan;94(1):43-50
18. Mitra M. *et al.* Fluorescence study of the effect of cholesterol on spectrin-aminophospholipid interactions. ***Eur Biophys J.*** 2015; 44: 635 – 645.
19. Halder S. *et al.*, Differential regulation of urine proteins in urothelial neoplasm. ***J Proteomics*** 2015; 127: 185 – 192.
20. Mitra M. *et al.*, Organization and dynamics of tryptophan residues in brain spectrin : Novel insight into conformational flexibility. ***J Fluorescence*** 2015; 25: 707 – 717.
21. Das D. *et al.*, Binding of hemin, hematoporphyrin and protoporphyrin with erythroid spectrin : fluorescence and molecular docking studies. ***Eur Biophys J.*** 2015; 44: 171-182.
22. Pahari BP *et al.*, Ground and excited state proton transfer of the bioactive plant flavonoid Robinetin in a protein environment: spectroscopic and molecular modelling studies. ***J. Phys. Chem. B.*** 2015; 119: 2533
23. Basak, N.P. and Banerjee S. Mitochondrial dependency in progression of acute myeloid leukemia. ***Mitochondrion*** 2015; 21:41-8.
24. Deb Pal A and Banerjee S. Epstein-Barr Virus latent membrane protein 2A mediated activation of Sonic Hedgehog pathway induces HLA class Ia downregulation in gastric cancer cells. ***Virology.*** 2015; 484:22-32.
25. Roy A and Banerjee S. p27 and Leukemia: Cell Cycle and Beyond. ***J Cell Physiol.*** 2015; 230(3):504-9.

2014

1. Kulkarni K.K *et al.*, Global gene expression profiling data analysis reveals key gene families and biological processes inhibited by Mithramycin in sarcoma cell lines. ***Genomics Data,*** 2014; 3:8-14.
2. Banerjee A *et al.*, Anticancer drug mithramycin interacts with core histones: an additional mode of action of the DNA groove binder. ***FEBS Open Bio.*** 2014; 4:987-995.
3. Banerjee A *et al.*, The DNA intercalators ethidium bromide and propidium iodide also bind to core histones. ***FEBS Open Bio.*** 2014; 4:251-9.
4. Bera K. *et al.*, A multicolor fluorescent peptide--nanoparticle scaffold: real time uptake and distribution in neuronal cells. ***New J. of Chemistry*** 2014; 38(7) 2739—2743.
5. Chakrabarti A *et al.*, Altered levels of amyloid precursor protein intracellular domain-interacting proteins in Alzheimer disease. ***Alzheimer Dis Assoc Disord.*** 2014; 28(3):283-90.
6. Chakrabarti A *et al.*, Differential expression of neuroblastoma cellular proteome due to AICD overexpression. ***J Alzheimers Dis.*** 2014; 38(4):845-55.
7. Roy K *et al.*, Growth factor receptor-bound protein 2 promotes autophagic removal of amyloid- β protein precursor intracellular domain overload in neuronal cells. ***J Alzheimers Dis.*** 2014; 38(4):881-95.

8. Roy K *et al*, Interaction of Grb2 SH3 domain with UVRAG in an Alzheimer's disease-like scenario. **Biochem Cell Biol.** 2014; 92(3):219-25.
9. Sengupta MB *et al*, CSF proteomics of secondary phase spinal cord injury in human subjects: perturbed molecular pathways post injury. **PLoS One.** 2014; 9(10):e110885
10. Baksi S *et al*, Mutant huntingtin replaces Gab1 and interacts with C-terminal SH3 domain of growth factor receptor binding protein 2 (Grb2). **Neurosci Res.** 2014; 87:77-83.
11. Roy S. *et al*, Equilibrium unfolding of cyclophilin from Leishmania donovani: characterization of intermediate states. **Int J Biol Macromol.** 2014; 69:353-60.
12. Vasudevarao M D *et al*, Naphthoquinone-mediated inhibition of lysine acetyltransferase KAT3B/p300, basis for non-toxic inhibitor synthesis. **J Biol Chem.** 2014; 289(11):7702-17.
13. Bera M *et al*, Characterization Of Unfolding Mechanism Of Human Lamin A Ig Fold By Single-Molecule Force Spectroscopy-Implications In EDMD. **Biochemistry.** 2014; 53(46):7247-58.
14. Srivastava D and Chakrabarti O. Mahogunin-mediated α -tubulin ubiquitination via noncanonical K6 linkage regulates microtubule stability and mitotic spindle orientation. **Cell Death and Disease** (2014), 5, e1064
15. Karmakar S. *et al.*, Differential proteomic study of platelets in asymptomatic constitutional macrothrombocytopenia: Altered levels of cytoskeletal proteins. **Eur J Haematol.** 2014; 94: 43-50.
16. Halder S. *et al.*, Differential regulation of few plasma proteins between members of a family with homozygous HbE and HbE β -thalassemia. **Thalassemia Reports.** 2014; 4(s1): 1837 (62 -64).
17. Saha S. *et al.*, Identification of Malignant B-lymphoblast Proteome De-regulations in B-cell Acute Lymphoblastic Leukemia. **EuPA Open Proteomics** 2014; 3: 13-26.
18. Patra M. *et al.*, Binding of polarity sensitive, hydrophobic ligands to erythroid and non-erythroid spectrin : Fluorescence and molecular modeling studies. **J Biomol Struct Dyn.** 2014; 32 (6): 852-865.
19. Roy A. *et al*, Molecular cross talk between Notch1, Shh and Akt pathways during erythroid differentiation of K562 and HEL cell lines. **Exp Cell Res.** 2014;320(1):69-78
20. Haldar, S. *et al.*, Differential regulation of MCM7 and its intronic miRNA cluster miR-19-106b-25 during megakaryopoiesis induced polyploidy. **RNA Biology** 2014; 11(9): 1137
21. Pal AD. *et al*, Epstein-Barr virus latent membrane protein-2A alters mitochondrial dynamics promoting cellular migration mediated by Notch signaling pathway. **Carcinogenesis.** 2014; 35(7):1592-601
22. Basak NP. *et al*, Alteration of mitochondrial proteome due to activation of Notch1 signaling pathway. **J Biol Chem.** 2014; 289(11):7320-34

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2. Chakrabarti A and D Mukhopadhyay BRAIN SENESCENCE-OMICS. **Journal of Proteins & Proteomics** 2013: 3(1), 15–29;
3. Bhattacharjee P *et al.*, Structural alterations of Lamin A protein in dilated cardiomyopathy. **Biochemistry.** 2013; 52 (24) :4229-41.

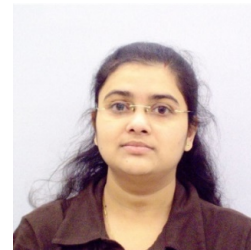
4. Ghosh S *et al.*, Ellipticine binds to a human telomere sequence: an additional mode of action as a putative anticancer agent? *Biochemistry*. 2013; 52(24):4127-37.
5. Ghosh S *et al.* Molecular basis of recognition of quadruplexes human telomere and c-myc promoter by the putative anticancer agent sanguinarine. *Biochim Biophys Acta*. 2013;1830(8):4189-201.
6. Banerjee A *et al.*, Fluorescence spectroscopic and calorimetry based approaches to characterize the mode of interaction of small molecules with DNA. *J. Fluoresc.* 2013;23(4):745-52.
7. Majumder P *et al.*, Minor groove binder distamycin remodels chromatin but inhibits transcription. *PLoS One*. 2013; 8(2):e57693. doi: 10.1371
8. Pal S and Dasgupta D. Differential scanning calorimetric approach to study the effect of melting region upon transcription initiation by T7 RNA polymerase and role of high affinity GTP binding. *J Biomol Struct Dyn*. 2013; 31(3):288-98.
9. Banerjee, A., *et al.*, Viscoelastic behavior of Human Lamin A proteins in the context of Dilated Cardiomyopathy . *PLoS One*. 2013; 8(12):e83410
10. Mukherjee R and Chakrabarti O. Mitochondrial quality control: decommissioning power plants in neurodegenerative diseases. *Scientific World J.*, 2013:180759
11. Chattopadhyay S, *et al.*, Identification of cellular calcium binding protein calmodulin as a regulator of rotavirus A infection during comparative proteomic study. *PLoS One*,2013, 8:e56655.
12. Chakrabarti A *et al.*, Differential thermal stability and oxidative vulnerability of the hemoglobin variants, HbA2 and HbE *PLoS One*. 2013;8(11)
13. Basu A. *et al.*, 2D DIGE based proteomics study of erythrocyte cytosol in sickle cell disease: altered proteostasis and oxidative stress. *Proteomics*. 2013; 13(21):3233-42.
14. Chakrabarti A. *et al.*, Erythrocyte membrane asymmetry in Thalassemia and Sickle Cell Disease. *Proc. Ind. Acad. Sci.* 2013; 79: 127-138.
15. Banerjee M, *et al.*, Interaction between Hemoglobin A and Merocyanine 540 : A spectroscopic investigation supported by docking. *Dyes & Pigments* 2013; 97: 446-454.
16. Sengupta B *et al.*, Prospect of Bioflavonoid Fisetin as a Quadruplex DNA Ligand: A Biophysical Approach, *PLOS One* 2013; 8:Art No: e65383
17. Chaudhuri S. *et al.*, Interactions of Dietary Flavonoids with Proteins: Insights from Fluorescence Spectroscopy and Other Related Biophysical Studies. *Curr. Drug Metabol.* 2013; 14: 491
18. Pahari B. *et al.*, Contrasting Binding of Fisetin and daidzein in γ -Cyclodextrin Nanocavity. *J. Photochem. Photobiol.* 2013; 118: 33-41
19. Roy A *et al.*, Increased cytoplasmic localization of p27(kip1) and its modulation of RhoA activity during progression of chronic myeloid leukemia. *PLoS One*. 2013;8(10):e76527. doi: 10.1371
20. Banerjee A. S. *et al.*, Epstein-Barr virus-encoded small non-coding RNAs induce cancer cell chemoresistance and migration. *Virology*. 2013;443(2):294-305.

2012

1. Ghosh S. et al., "Patch"-ing up the neurons: revival or enervation? *Vitam Horm.* 2012;88:439-59.
2. Raychaudhuri M. et al., The N-terminal SH3 domain of Grb2 is required for endosomal localization of A β PP. *J Alzheimers Dis.* 2012; 32(2):479-93.
3. Chakrabarti A and Mukhopadhyay D. Novel adaptors of amyloid precursor protein intracellular domain and their functional implications. *Genomics Proteomics Bioinformatics.* 2012;10(4):208-16.
4. Das S. et al., Biophysical studies with AICD-47 reveal unique binding behavior characteristic of an unfolded domain *Biochem Biophys Res Commun.* 2012;425(2):201-6.
5. Bhowmick R. et al., Rotaviral enterotoxin nonstructural protein 4 targets mitochondria for activation of apoptosis during infection. *J. Biol. Chem.*, 287, 35004-35020.
6. Dasgupta D. et al, A revisit of the mode of interaction of small transcription inhibitors with genomic DNA. *J Biosci.* 2012; 37(3):475-81.
7. Pal S. et al., Structural studies of arginine induced enhancement in the activity of T7 RNA polymerase. *Biochem Biophys Res Commun.* 2012; 421(1):27-32.
8. Lahiri S. et al., Association of aureolic acid antibiotic, chromomycin A3 with Cu²⁺ and its negative effect upon DNA binding property of the antibiotic. *Biometals.* 2012; 25(2):435-50.
9. Banerjee M et al., Interaction of Merocyanine 540 with serum albumins : Photophysical and Binding studies. *J. Photochem. Photobiol. B.* 2012; 108: 23-33.
10. Ghosh M and A. K Pal, Radioprotection imparted by four spices in a bacterial system, *Pharmacognosy Comm.* 2012; 2: 42
11. Banerjee M. et al., Oxidative interaction between oxyHb and ATP : A Spectroscopic Study. *J Phy Chem B.* 2012; 116: 6150-6157.
12. Saha S. et al., Fractional precipitation of plasma proteome by ammonium sulphate: case studies in leukemia and thalassemia. *J Proteomics Bioinformatics* 2012; 5: 163-171.
13. Pahari B et al., Binding and antioxidant properties of therapeutically important plant flavonoids in biomembranes: insights from spectroscopic and quantum chemical studies *Chem Phys Lipids.* 2012; 165(4):488-96
14. Chakraborty S. et al., A critical study on the interaction of Hesperitin with human hemoglobin: Fluorescence spectroscopy and molecular modelling approach. *J Lumin.* 2012;132(6):1522-1528
15. Das D. et al., Identical RNA-protein interactions in vivo and in vitro and a scheme of folding the newly synthesized proteins by ribosomes. *J Biol Chem.* 2012; 287(44):37508-21.
16. Roy A. et al., Notch1 intracellular domain increases cytoplasmic EZH2 levels during early megakaryopoiesis. *Cell Death and Disease.* 2012; 3: e380. doi: 10.1038/cddis.2012.119

Biosketch

Chandrima Das, PhD
Associate Professor-E



Education:

- Ph.D. (2007) with specialization in Chromatin Biology from Jawaharlal Nehru Centre for advanced Scientific Research (JNCASR), Bangalore, India.
- M.Sc. (2001) in Biochemistry, University of Calcutta, Kolkata, India.
- B.Sc. (1999) in Chemistry, University of Calcutta, Kolkata, India.

Academic Positions:

- 2012-Present: Associate Professor E, Saha Institute of Nuclear Physics
- 2010 - 2012: Postdoctoral Fellow, Department of Biochemistry and Molecular Biology, MD. Anderson Cancer Center, TX, USA.
- 2008 - 2010: Postdoctoral Fellow, Department of Molecular Biology, University of

Awards/Honors:

- *Ramalingaswami Fellowship from Department of Biotechnology (2012-2017).*
- Susan G. Komen Postdoctoral Fellowship awarded for basic sciences in Breast Cancer Research (2009-2012).
- Life Member of Society of Biological Chemists (SBC), India (2007).
- Life Member of Chemical Biology Society (CBS), India (2016).
- Life Member of Indian Society of Cell Biology (ISCB), India (2017).
- Life Member of Indian Association for Cancer Research (IACR), India (2017).

Field of Specialization:

Research in Chromatin Dynamics Laboratory at SINP focus on the modulation of chromatin structure by a ubiquitous class of proteins called “*readers/effectors*” which has become an important paradigm in chromatin biology. Binding of these chromatin readers recruits or stabilizes various other factors affecting all the essential DNA-templated processes including transcription, repair, recombination and replication. We are trying to understand the ability of these readers to dictate the “on” or “off” state of the underlying genes and their aberrant epigenetic recognitions leading to diseases including cancer.

List of Publications (2012- 2017):

Chromatin Readers/Effectors as novel signaling platforms:

1. Basu M, Sengupta I, Khan W, Srivastava DK, Chakrabarti P, Roy S, **Das C***. Dual histone reader ZMYND8 inhibits cancer cell invasion by positively regulating epithelial genes. *Biochem J*. 2017, 474(11):1919-1934.
2. Basu M, Khan MW, Chakrabarti P, **Das C***. Chromatin reader ZMYND8 is a key target of all trans retinoic acid-mediated inhibition of cancer cell proliferation. *Biochim Biophys Acta- Gene Regulatory Mechanisms*. 2017, 1860(4):450-459.
3. Adhikary S, Sanyal S, Basu M, Sengupta I, Sen S, Srivastava DK, Roy S*, **Das C***. Selective Recognition of H3.1K36 dimethylation / H4K16 acetylation facilitates the regulation of ATRA-responsive genes by putative chromatin reader ZMYND8. *J Biol Chem*. 2016, 291:2664-81.
4. Chakrabarti R, Sanyal S, Ghosh A, Bhar K, **Das C*** and Siddhanta A*. Phosphatidylinositol 4-phosphate 5-kinase 1-alpha modulates ribosomal RNA gene silencing through its interaction with histone H3 lysine 9 trimethylation and heterochromatin protein HP1-alpha. *J Biol. Chem*. 2015, 290:20893-903.
5. **Das C**, Roy S, Namjoshi S, Malarkey CS, Jones DN, Kutateladze TG, Churchill ME, Tyler JK. Binding of the histone chaperone ASF1 to the CBP bromodomain promotes histone acetylation. *Proc Natl Acad Sci U S A*. 2014, 111(12):E1072-81.

Epigenetic alterations of host genome during viral infection:

1. Das D, Sengupta I, Sarkar N, Pal A, Saha D, Bandopadhyay M, **Das C**, Narayan J, Singh SP, Chakrabarti S, Chakravarty R. Anti-hepatitis B virus (HBV) response of imiquimod based toll like receptor 7 ligand in hbv-positive human hepatocellular carcinoma cell line. *BMC Infect Dis*. 2017, 17(1):76.
2. Das D, Sarkar N, Sengupta I, Pal A, Saha D, Bandopadhyay M, **Das C**, Narayan J, Singh SP, Chakravarty R. Anti-viral role of toll like receptor 4 in hepatitis B virus infection: An *in vitro* study. *World J Gastroenterol*. 2016, 22(47):10341-10352.
3. Bandopadhyay M, Sarkar N, Datta S, Das D, Pal A, Panigrahi R, Banerjee A, Panda CK, **Das C**, Chakrabarti S, Chakravarty R. Hepatitis B virus X protein mediated suppression of miRNA-122 expression enhances hepatoblastoma cell proliferation through cyclin G1-p53 axis. *Infect Agent Cancer*. 2016 Aug 15;11:40.

Small molecule modulators as epigenetic regulators:

1. Goswami S, Sanyal S, Chakraborty P, **Das C***, Sarkar M*. Interaction of a Common Painkiller Piroxicam and Copper-piroxicam with Chromatin Causes Structural Alterations Accompanied by Modulation at the Epigenomic/Genomic level. **Biochim Biophys Acta- General Subjects**. 2017, 4165(17)30131-9.
2. Banerjee A, Sanyal S, Dutta S, Chakraborty P, Das PP, Jana K, Vasudevan M, **Das C***, Dasgupta D*. The plant alkaloid chelerythrine binds to chromatin, alters H3K9Ac and modulates global gene expression. **Journal of Biomolecular Structure and Dynamics**. 2016, 5:1-9.
2. Banerjee A, Sanyal S, Majumder P, Chakraborty P, Jana K, **Das C***, Dasgupta D*. Recognition of chromatin by the plant alkaloid, ellipticine as a dual binder. **Biochem Biophys Res Commun**. 2015, 462:352-7.
3. Kulkarni K.K., Bankar K.G., Shukla R.N., **Das C**, Banerjee A, Jana K, Dasgupta D, Vasudevan M. Global gene expression profiling data analysis reveals key gene families and biological processes inhibited by Mithramycin in sarcoma cell lines. **Genomics Data**, 2014, 3:8-14.
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5. Banerjee A, Majumder P, Sanyal S, Singh J, Jana K, **Das C***, Dasgupta D*. The DNA intercalators ethidium bromide and propidium iodide also bind to core histones. **FEBS Open Bio**. 2014, 4:251-9.

Reviews & Book Chapters:

1. Mukherjee S, Adhikary S, Roy S, **Das C***. Noncoding RNAs as chromatin scaffold of histone modification complexes in cancer. 2017. Cancer and Non coding RNAs, Translational Epigenetics Series. (In Press)
2. Kumari S, **Das C**, Sikder S, Kumar M, Bachu M, Ranga U, Kundu TK. Identification and characterization of nonhistone chromatin proteins: human positive coactivator 4 as a candidate. **Methods Mol Biol**. 2015, 1288: 245-72.
3. **Das, C.**, and Tyler, J.K. Histone exchange and histone modifications during transcription and aging. **Biochim Biophys Acta**. 2013, 1819(3-4): 332-42.

* Corresponding author

List of Conferences attended as Invited Speakers (2012- Present):

1. 15th Asian Conference on Transcription (ACT-XV)", 2017 at Penang, Malaysia. (An upcoming event)
2. (a) 6th Meeting of the Asian Forum for Chromatin and Chromosome Biology, 2017 at CCMB, Hyderabad, (b) 5th Meeting of the Asian Forum for Chromatin and Chromosome Biology, 2015 at JNCASR, Bangalore.
3. 11th Asian Epigenomics Meeting, 2016 at JNCASR, Bangalore.
4. (a) 17th Transcription Assembly Meeting, 2014 at JNCASR, Bangalore, (b) 16th Transcription Assembly Meeting, 2013 at Vedic Village, Kolkata.
5. (a) 6th Ramalingaswami Conclave, 2017 at IISER, Pune, (b) 4th Ramalingaswami Conclave, 2015 at Institute of Life Sciences, Nalco Square Bhubaneswar.

Joint Conference Organizer of National Meetings (2012- Present):

1. "19th Transcription Assembly Meeting" organized by Bose Institute in association with SINP and IICB, Kolkata, 2016.
2. "National Symposium on Frontiers of Biology: The DAE Spectra" organized by SINP, 2015.
3. "Biomolecular Recognition and Chemical Biology" organized by SINP, 2013.

Ongoing Research Projects:

- Chromatin dynamics and its modulation by transcription factors funded by **DAE** (Intramural). Duration: 2012-2017
- Prolyl Isomerization as a novel mode to regulate chromatin function funded by Ramalingaswami Fellowship (**DBT**). Duration: 2012 – 2017
- A putative chromatin reader ZMYND8 and its role in neuronal differentiation by **DST-SERB**. Duration: 2015-2018.

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Educational Background

2000 University of Calcutta Kolkata, India.

Ph.D. in Biophysics, Molecular Biology and Genetics (*awarded in 2001*)

1995 University of Calcutta Kolkata, India.

M.Sc. in Biophysics and Molecular Biology (First Class)

1993 University of Calcutta Kolkata, India.

B.Sc. in Physics (First Class)

Academic Positions

2016–till date: Professor 'G', Biophysics & Structural Genomics Division;

2011-2016: Associate Professor 'F', Structural Genomics Division,

2007-2010: Associate Professor 'E', Structural Genomics Section;

2005-2007: Reader 'D', Structural Genomics Section;

2003-2005: Research Scientist, School of Medicine, University of California at San Diego, USA

2000–2003: Research Associate, Dept of Mol & Exp Medicine, The Scripps Research Institute, USA

Awards/ Honours

DST-SERB International Travel Grant (2017)

Co-PI, DBT – NE Twinning Project (2016 – 2019)

Associate Editor, Journal of Alzheimer's Disease, IOS Press, Fairfax, USA.

Editor, Journal of Proteins and Proteomics, India.

Skagg's Post-doctoral Research Fellowship (2001 – 2003)

Research Focus

- Molecular players in Neurodegenerative Diseases like Alzheimer's and Huntington Disease– adaptor Protein (viz., Grb2) Interactions
- Modeling of Molecular & Pathway Cross-talk in Neurodegenerative Diseases
- Understanding AICD mediated Cellular Dynamics, Trafficking and Cytotoxicity
- Protein Interactions in Regeneration – Spinal Cord Injury & Neuromyelitis Optica Proteomics

Research Guidance/ Publication Statistics

No. of Ph.D. students supervised: 10 (6 received Ph.D. degree); co-supervised: 2 (1 received Ph.D. degree)

No. of Research Associates mentored: 02

No. of papers in peer-reviewed journals: 45 and in selected proceedings: 12

Publications (2012-2017)

1. Majumder P, Roy K, Singh BK, Jana NR, Mukhopadhyay D. Cellular levels of growth factor receptor bound protein 2 (Grb2) and cytoskeleton stability are correlated in a neurodegenerative scenario. *Dis Model Mech.* 2017 Mar 30.
2. Sengupta MB, Saha S, Mohanty PK, Mukhopadhyay KK, Mukhopadhyay D. Increased expression of ApoA1 after neuronal injury may be beneficial for healing. *Mol Cell Biochem.* 2017 Jan;424(1-2):45-55.

3. Baksi S, Bagh S, Sarkar S, Mukhopadhyay D. Systemic study of a natural feedback loop in Huntington's disease at the onset of neurodegeneration. *Biosystems*. 2016 Dec;150:46-51.
4. Sengupta MB, Mukhopadhyay D. Possible role of apolipoprotein A1 in healing and cell death after neuronal injury. *Front Biosci (Elite Ed)*. 2016 Jun 1;8:460-77.
5. Sengupta MB, Chakrabarti A, Saha S, Mukhopadhyay D. Clinical proteomics of enervated neurons. *Clin Proteomics*. 2016 May 5;13:10.
6. Chaperone-like protein HYPK and its interacting partners augment autophagy. K Roy Chowdhury, S Baksi, Bucha S, Mukhopadhyay D, Bhattacharyya NP. *European Journal of Cell Biology* (2016), 2016 Jun-Jul;95(6-7):182-94.
7. Regulation of mitochondrial morphology and cell cycle by microRNA-214 targeting Mitofusin2. Bucha S, Mukhopadhyay D, Bhattacharyya NP. *Biochem Biophys Res Commun*. 2015 Oct 2;465(4):797-802.
8. A multicolor fluorescent peptide--nanoparticle scaffold: real time uptake and distribution in neuronal cells. Bera Kallol, Baksi Shounak, Nag Moupriya, Bera Subhas Chandra, Mukhopadhyay Debashis and Basak Soumen. *New Journal of Chemistry* (2014), 38,(7), 2739—2743.
9. Chakrabarti A, Chatterjee A, Sengupta MB, Chattopadhyay P, Mukhopadhyay D. Altered levels of amyloid precursor protein intracellular domain-interacting proteins in Alzheimer disease. *Alzheimer Dis Assoc Disord*. 2014 Jul-Sep;28(3):283-90.
10. Chakrabarti A, Roy K, Mukhopadhyay D. Differential expression of neuroblastoma cellular proteome due to AICD overexpression. *J Alzheimers Dis*. 2014;38(4):845-55.
11. Roy K, Raychaudhuri M, Chakrabarti O, Mukhopadhyay D. Growth factor receptor-bound protein 2 promotes autophagic removal of amyloid- β protein precursor intracellular domain overload in neuronal cells. *J Alzheimers Dis*. 2014;38(4):881-95.
12. Baksi S, Jana NR, Bhattacharyya NP, Mukhopadhyay D. Grb2 is regulated by foxd3 and has roles in preventing accumulation and aggregation of mutant huntingtin. *PLoS One*. 2013 Oct 8;8(10):e76792.
13. Roy K, Chakrabarti O, Mukhopadhyay D. Interaction of Grb2 SH3 domain with UVRAG in an Alzheimer's disease-like scenario. *Biochem Cell Biol*. 2014 Jun;92(3):219-25.
14. Sengupta MB, Basu M, Iswarari S, Mukhopadhyay KK, Sardar KP, Acharyya B, Mohanty PK, Mukhopadhyay D. CSF proteomics of secondary phase spinal cord injury in human subjects: perturbed molecular pathways post injury. *PLoS One*. 2014 Oct 28;9(10):e110885
15. Baksi S, Basu S, Mukhopadhyay D. Mutant huntingtin replaces Gab1 and interacts with C-terminal SH3 domain of growth factor receptor binding protein 2 (Grb2). *Neurosci Res*. 2014 Oct;87:77-83.
16. BRAIN SENESCENCE-OMICS. A Chakrabarti, D Mukhopadhyay. *Journal of Proteins & Proteomics* 3 (1), 15 – 29, 2013.
17. Ghosh S, Chakrabarti A, Mukhopadhyay D. "Patch"-ing up the neurons: revival or enervation? *Vitam Horm*. 2012;88:439-59.
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19. Das S, Ghosh S, Dasgupta D, Sen U, Mukhopadhyay D. Biophysical studies with AICD-47 reveal unique binding behavior characteristic of an unfolded domain. *Biochem Biophys Res Commun*. 2012 Aug 24;425(2):201-6.
20. Chakrabarti A, Mukhopadhyay D. Novel adaptors of amyloid precursor protein intracellular domain and their functional implications. *Genomics Proteomics Bioinformatics*. 2012 Aug;10(4):208-16.

Teaching Experience

Post-MSc teaching in SINP on Molecular Genetics, Neurobiology and Biophysics; Postgraduate teaching in University of Calcutta (Biochemistry, Biotechnology, Neurosciences, Microbiology, Genetics, Biophysics and Molecular Biology) and St Xaviers College, Kolkata on X-ray Crystallography, Mass Spectrometry; Postgraduate teaching in NIPER, Kolkata on Molecular Modelling.



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Education

Postdoctoral Research Fellow at Northwestern University, Chicago, USA (2004-2010)
Ph. D in Biochemistry from International Max Planck Research School, J.W. Goethe University of Frankfurt, Germany (2001-2004)
M. Tech. in Bio-medical Engineering from Indian Institute of Technology (IIT), Bombay, India (2000)
M. Sc in Biochemistry from University of Calcutta, Kolkata, India (1998)
B. Sc (Honors) in Chemistry from University of Calcutta, Kolkata, India (1996)

Academic positions

2016- Present: Associate Professor – F, Biophysics & Structural Genomics Division (SINP)
2010-2016 Associate Professor–E, Biophysics & Structural Genomics Division (SINP)

Awards & Honors

1. DBT-CREST Award for Stem Cell Research & Regenerative Medicine (2012)
2. BAT/Ila Ph.d Fellowship from International Max Planck Research School in Germany (2001-2004)
3. GATE Fellowship (1998) for All India Rank 2 in India
4. Shanti Bhakta Memorial Award (1996), in India
5. National Merit Scholarship (1991) in India

Thesis Supervised

Serial No.	Name	Title	Duration	Postdoc
1.	Ms. Avinanda Banerjee	Effects of Lamin A mutations in nuclear morphology, function and mechanics-A plausible link with dilated Cardiomyopathy	2010-2015	NCBS
2.	Ms. Pritha Bhattacharjee	Mechanistic elucidation of the role of Lamin A in dilated Cardiomyopathy	2010-2015	CNRS France
3.	Mr. Manindra Bera	Biomechanics of human lamin A in the light of muscular dystrophy	2011-2016	Rockefeller University

Areas of Expertise

Publications

1. Bhattacharjee, P., Banerjee, A., Banerjee, A., Dasgupta, D. and **Sengupta, K. (2013)** Biophysical Characterization of Dilated Cardiomyopathy related lamin A Mutants. **Biochemistry**, Jun 18;52(24): 4229-41.
2. Banerjee, A., Rathee, V., Krishnaswamy, R., Bhattacharjee, P., Ray, P., Sood, A.K. and **Sengupta, K (2013)** Viscoelastic behavior of Human Lamin A proteins in the context of Dilated Cardiomyopathy . **PLoS One. 2013 Dec 30;8(12):e83410**
3. Bera M, Kotamarthi Hc, Dutta S, Ray A, Ghosh S, Bhattacharyya D, Ainaravaru Sr, **Sengupta K (2014)** Characterization Of Unfolding Mechanism Of Human Lamin A Ig Fold By Single-Molecule Force Spectroscopy-Implications In EDMD. **Biochemistry**. Nov 25;53(46):7247-58.
4. BANERJEE, A., GHOSHAL, P.K. & **SENGUPTA, K (2015)** NOVEL LINKAGE OF *LMNA* SINGLE NUCLEOTIDE POLYMORPHISM WITH DILATED CARDIOMYOPATHY IN AN INDIAN CASE STUDY. **IJC HEART & VASCULATURE**. JUNE: **7**: 99-105.
5. Roy J, Mitra S, **Sengupta K**, Mandal AK **(2015)** Hsp70 clears misfolded kinases that partitioned into distinct quality-control compartments. **Mol Biol Cell**. May 1;26(9):1583-600.
6. Bhattacharjee, P., Dasgupta, D. and **Sengupta, K. (2015)** Molecular Events in Lamin B1 Homopolymerization: A Biophysical Characterization. **The Journal of Physical Chemistry Part B: Nov 5;119(44):14014-21**
7. Bera M, Ainaravaru SR & **Sengupta K. (2016)** Significance of 1B and 2B domains in modulating elastic properties of lamin A. **Sci Rep**. 2016 Jun 15;6:27879
8. Dutta, S., Bhattacharyya, M. & Sengupta, K **(2016)** Implications and assessment of the elastic behavior of lamins in laminopathies. *Cells* 5(4) 37
9. Dey SK, Singh RK, Chatteraj S, Saha S, Das A, Bhattacharyya K, **Sengupta K**, Sen S, **Jana SS.** (2017) Differential role of nonmuscle myosin II isoforms during blebbing of MCF-7 cells. **Mol Biol Cell**. Mar 1. pii: mbc.E16-07-0524. doi: 10.1091/mbc.E16-07-0524. [Epub ahead of print]

Conferences / Symposia/Workshops attended mentioning the employee's own role in it.

- Invited talk at IABS 2015, Indian Association for the Cultivation of Science, Feb 2-3, 2015
- Invited talk at National Symposium on Biophysics & Golden Jubilee Meeting of the Indian Biophysical Society, Jamia Millia Islamia, Feb 14-17, 2015
- Invited expert for Nikon Imaging workshop at NCBS, Bangalore, Nov, 2015
- Invited speaker at the OWLS, TIFR, Feb, 2016 (declined)
- Invited speaker at 11TH International Symposium on Cell Surface Macromolecules, IISER Mohali, Feb 24-28, 2017
- Invited speaker at Emerging Trends in Biology- Symposium , Calcutta University, 17th March, 2017

Teaching/ Lectures delivered

Teaching Molecular Biology (Transcription) and Advanced Cell Biology (Cell motility, biopolymers, mechanotransduction), Confocal Microscopy and super resolution imaging in post M.Sc teaching coursework
Invited Lecture series at IISER, Kolkata 8th May, 2016

Oishee Chakrabarti, PhD
Associate Professor F



Academic qualification: Ph D, National Centre for Biological Sciences (NCBS), TIFR, Bangalore, 2003

Positions held (in chronological order)

<i>Year (s)</i>	<i>University / Institution</i>	<i>Positions held</i>
2003-2004	NCBS, TIFR, Bangalore	Postdoctoral Fellow
2004-2005	Harvard Medical School	Postdoctoral Fellow
2005-2009	NICHD, National Institutes of Health	Postdoctoral Fellow
2010-2016	Saha Institute of Nuclear Physics	Associate Professor "E"
2016-till date	Saha Institute of Nuclear Physics	Associate Professor "F"

Research highlights:

Ongoing research in my laboratory very elegantly demonstrates that while trying to understand the actual cell biology behind extensive cellular dysfunction and death as evidenced in late-onset neurodegenerative diseases, we have unravelled some basic mechanisms that regulate organellar biogenesis and in turn their function.

The Prion protein (PrP) is a highly conserved cell surface glycoprotein implicated in several neurodegenerative diseases such as scrapie, bovine spongiform encephalopathy, Creutzfeldt-Jakob disease and Gerstmann-Straussler-Scheinker disease. The pathogenesis of prion diseases requires its expression and is often accompanied by the presence in brain of one or more abnormal isoforms of the prion protein (PrP). Presumably, the aberrant protein species can engage in atypical interactions and ultimately leads to a series of unknown events culminating in cell death, as has been recently demonstrated for some of the disease causing isoforms of PrP and their interactions with the cytosolic E3 ligase, Mahogunin RING finger1 (MGRN1). The mechanisms leading to disease are not fully understood, but it is plausible to hypothesize that in addition to the gain of new toxic properties of PrP isoforms, loss of wild-type function of prion-interacting proteins also contributes to pathogenesis.

One such example would be functional inactivation of MGRN1, affecting a plethora of cellular pathways – the fusion between MVB/amphisome and lysosome, the mitochondrial fission-fusion dynamics. It also affects tubulin polymerisation, which in turn regulates spindle orientation during cell division and intra-cellular cargo transport in interphase cells.

Future plans:

- Establish ERAD tuning and how it regulates ER-mitochondria interactions and maintains intracellular membrane architecture under physiological and pathological conditions, like glioblastoma, neurodegenerative diseases, exposure to drugs and irradiation.
- Identify, characterize and establish the microRNAs that regulate ER stress and thereby play significant role in ERAD tuning in pathologies of the brain – glioblastoma and neurodegeneration.
- Mapping the mega-architectural changes at the cellular level that occur during the progression of glioblastoma and lesser studied neuropathies.
- Establish potential intracellular drug targets that tilt the balance between cancer and neurodegeneration.

Publications (2012-2017):

1. Kaul Z and **Chakrabarti O**. Tumor susceptibility gene 101, TSG101, regulates predisposition towards apoptosis via ESCRT machinery accessory proteins. *Molecular Biology of the Cell*, epub ahead of print, doi: 10.1091/mbc.E16-12-0855 (2017)
2. Majumder P and **Chakrabarti O**. Lysosomal quality control in Prion diseases. *Molecular Neurobiology*, epub ahead of print, doi: 10.1007/s12035-017-0512-8 (2017)
3. Mukherjee R, Das A, Chakrabarti S and **Chakrabarti O**. Calcium dependent regulation of protein ubiquitination – interplay between E3 ligases and calcium binding proteins. *Biochimica et Biophysica Acta (BBA) - Molecular Cell Research*, 1864, 1227-1235 (2017).
4. Mukherjee M and **Chakrabarti O**. Regulation of Mitofusin1 by Mahogunin Ring Finger-1 and the proteasome modulates mitochondrial fusion. *Biochimica et Biophysica Acta (BBA) - Molecular Cell Research*, 1863, 3065-3083 (2016).
5. Bera K, Sau A, Mondal P, Mukherjee R, Mookherjee D, Metya A, Kundu AK, Mandal D, Satpati B, **Chakrabarti O**, and Basu S. Metamorphosis of Ruthenium Doped Carbon Dots: In Search for Origin of Photoluminescence and Beyond. *Chemistry of Material*, 28, 7404–7413 (2016).
6. Srivastava D, Mukherjee R, Mookherjee D and **Chakrabarti O**. Mahogunin mediated regulation of G α _i localisation during mitosis and its effect on spindle positioning. *Biochemistry and Cell Biology*, 94, 359-69 (2016).
7. Majumder P and **Chakrabarti O**. ESCRTs and associated proteins in lysosomal fusion with endosomes and autophagosomes. *Biochemistry and Cell Biology*, epub ahead of print, 1-8 (2016).
8. Mukherjee R and **Chakrabarti O**. Ubiquitin mediated regulation of the E3 ligase GP78 by Mahogunin in trans affects mitochondrial homeostasis. *Journal of Cell Science*. pii: jcs.176537 (2016).
9. Majumder P and **Chakrabarti O**. Mahogunin regulates fusion between amphisomes/MVBs and lysosomes via ubiquitination of TSG101. *Cell Death and Disease*, 6, e1970 (2015).
10. Srivastava D and **Chakrabarti O**. Ubiquitin in regulation of spindle apparatus and its positioning: implications in development and disease. *Biochemistry and Cell Biology*, 93, 273-281 (2015).
11. Theeya N, Ta A, Das S, Mandal RS, **Chakrabarti O**, Chakrabarti S, Ghosh AN, Das S. An inducible and secreted eukaryote-like serine/threonine kinase of Salmonella enterica serovar Typhi promotes intracellular survival and pathogenesis. *Infection and Immunity*, 83, 522-533 (2015).
12. Roy K, **Chakrabarti O**, Mukhopadhyay D. Interaction of Grb2 SH3 domain with UVRAG in an Alzheimer's disease-like scenario. *Biochemistry and Cell Biology*, 92, 219-225 (2014).
13. Srivastava D and **Chakrabarti O**. Mahogunin-mediated α -tubulin ubiquitination via noncanonical K6 linkage regulates microtubule stability and mitotic spindle orientation. *Cell Death and Disease*, 5, e1064 (2014).
14. Roy K, Raychaudhuri M, **Chakrabarti O** and Mukhopadhyay D. Growth factor receptor-bound protein 2 promotes autophagic removal of amyloid- β protein precursor intracellular domain overload in neuronal cells. *Journal of Alzheimer's Disease*, 38, 881-895 (2014).
15. Mukherjee R and **Chakrabarti O**. Mitochondrial quality control: decommissioning power plants in neurodegenerative diseases. *ScientificWorldJournal*, 2013:180759 (2013).
16. Chattopadhyay S, Basak T, Nayak MK, Bhardwaj G, Mukherjee A, Bhowmick R, Sengupta S, **Chakrabarti O**, Chatterjee NS and Chawla-Sarkar M. Identification of cellular calcium binding protein calmodulin as a regulator of rotavirus A infection during comparative proteomic study. *PLOS One*, 8:e56655 (2013).
17. Bhowmick R, Halder UC, Chattopadhyay S, Chanda S, Nandi S, Bagchi P, Nayak MK, **Chakrabarti O**, Kobayashi N and Chawla-Sarkar M. Rotaviral enterotoxin nonstructural protein 4 targets mitochondria for activation of apoptosis during infection. *Journal of Biological Chemistry*, 287, 35004-35020 (2012).

Sangram Bagh, PhD
Associate Professor-E
Ramanujan Fellow



Education

PhD (Chemistry) **University of Toronto**, Toronto, Canada 2010
MS (Chemistry), **University of Saskatchewan**, Canada 2005
B.Tech (Petrochemicals and Petroleum Refinery Engineering), **University of Calcutta**, 2002
B.Sc Chemistry (Honors), **Burdwan University** 1999

Academic Position

Associate Professor-E, Biophysics and Structural Biology Division, **Saha Institute Of Nuclear Physics**, Kolkata, India, September 2014- Present
Assistant Professor in Biotechnology, **Presidency University** June 2013- September 2014
Post Doctoral Research, Chemical Engineering, **Massachusetts Institute of Technology (MIT)**, USA (2011-2013)

Awards and Scholarships

2017 WOS Travel Award, SB7.0, Singapore
2015-2020 Ramanujan Fellowship, Govt. of India
2010-2012 NSERC Postdoctoral Fellowship, Department of Chemical Engineering, MIT
2010-2011 Postdoctoral Fellowship, Department of Chemical Engineering, MIT(declined)
2010 F.E. Beamish Prize in Physical Chemistry, Dept. of Chemistry, University of Toronto
2009-2010 F.E. Beamish Graduate Scholarship in Science and Technology, Govt. of Ontario
2009-2010 Pfizer Graduate Scholarship in Science and Technology (declined)
2009 Donald J. LeRoy Prize for research excellence, University of Toronto
2009 Travel Award, International Workshop on Bio-Design Automation, San Francisco, CA
2008 ICSB travel award, Systems Biology Organization, Gothenburg, Sweden
2008 BioBricks Foundation SB4.0 Travel Award, Hong Kong (declined)
2010, 2008 RGO conference travel award, UTM (2 times recipient)
2007 CRM travel award, University of Montreal, Montreal, Canada
2007 University of Toronto Conference Travel Award (Department of Chemistry)
2006 MITACS Travel award, Montreal
2003-2005 Arts and Science Fellowship, University of Saskatchewan
1999-2002 National Merit Scholarship of Govt. of India, University of Calcutta

Research (2012-2017)

I have joined this institute little more than 2 years back to start a synthetic biology lab. Synthetic biology is new field of bioengineering where electrical engineering principles are adapted in molecular biology to reprogram new cellular functions predictively. It has potential to solve thrust problems in medicine, energy, materials and space exploration, which cannot be achieved by conventional genetic engineering. This field is very new in India and our new lab has three research focuses.

i) **Space synthetic and systems biology:** We have recently established a systems biology pipeline and analyze the effect of microgravity on global gene expression data of human and bacterial cells from space and simulated microgravity experiments. We have found multiple new pathways, network and new insight, which were not possible by conventional analysis. This study indicates to some new disease signatures in microgravity, including few types of cancers, may help assessing risks of long duration space travel and developing new space medicine. The works also suggest plausible molecular reasoning for previously unexplained facts related to space travel including the altered smelling behaviour of astronauts, the increased survival of salmonella in macrophages in microgravity and deregulation upstream signalling pathways in immunity. The works are

published in Scientific Reports and Astrobiology (**highlighted as high impact article by editorial board**) and featured in *Nature India*, *Times of India* and our institutional homepage.

ii) **Complex gene circuits for cellular computation**: Creating human designed complex computation in living cell is a key challenge in synthetic biology. Here we are developing electronic analog of 2-to-4 biochemical decoder, 4-to-2 encoder, multiplexer and de-multiplexer, tunable verticle scaller using synthetic gene circuits in *E.coli*.

Future: We will continue all the directions we have proposed. We will further create a synthetic biology platform technology for programmed and autonomous delivery of RNAi into cancer cells.

Research Publications (2012-2017)

1. Roy R, Shilpa P.P and **Bagh S*** (2016) A systems biology analysis unfolds the molecular pathways and networks of pathogenic bacteria in space flight and simulated microgravity condition, *Astrobiology*, 16, 677–689 * corresponding author (**This work is highlighted as a high impact article by the editorial board of the Astrobiology**)

2. Baksi S., **Bagh S**, Sarkar S. and Mukhopadhyay D. (2016) Systemic study of a natural feedback loop in Huntington's disease at the onset of neurodegeneration. *Biosystems* 150, 46-51.

3. Mukhopadhyay S, Saha R, Palanisamy A, Ghosh M, Biswas A, Roy S, Pal A, Sarkar K and **Bagh S*** (2016) A systems biology pipeline identifies new immune and disease related molecular signatures and networks in human cells during microgravity exposure, *Scientific Reports*, 6:25975, DOI: 10.1038/srep25975, * corresponding author. (**This work is highlighted in Nature India**, May 2016, Times of India and SINP Homepage)

4. **Bagh S***, (2016) Reprogramming living cells with an engineering language, *Physics News*, 46, 43-52

5. Love K, **Bagh S**, Choi J, and Love J.C. (2013) Microtools for single-cell analysis in biopharmaceutical development and manufacturing, *Trends in Biotechnology*, 31, 280-286

Invited Talks

2017 JC Bose Trust Lecture, JC Bose Heritage Museum, Kolkata

2017 International Synthetic Biology Conference, Singapore (contributed talk)

2017 International Biological Engineering Meeting, JNU, Delhi

2017 Theoretical and Computational Material Science Seminar Series, SNBNCBS, Kolkata

2017 Transcriptional Assembly Meeting, Bose Institute, Kolkata

2016 AJC Bose Lecture, IEST, Shibpur

2016 Biological Sciences Colloquium, Presidency University

2016, NNMCB National Meeting, IISER-Pune, Pune

2016, DBT Workshop on Physics in Biology, St. Xavier's College, Kolkata

2015, Frontiers in Biology: DAE Spectra, SINP, Kolkata

2014, Indo-US workshop on Synthetic Biology, New Delhi

2014, ICEBEM-2014, Santiniketan

2012, Department of Biological Sciences and Biological Engineering, Indian Institute of Technology (IIT) Kanpur, India

2012, Department of Biological Chemistry, Indian Association for the Cultivation of Science, Kolkata, India

2012, Department of Chemical Engineering, Indian Institute of Science (IISc) Bangalore, India

2010, Department of Systems Biology, Harvard Medical School, Boston, USA

2010, FAS Center of Systems Biology, Harvard University, Cambridge, USA

2010, LeRoy Award Lecture, Department of Chemistry, University of Toronto, Canada

PhD Student Guidane: Two students are working in my supervision

Teaching and New Course Development (2012-2017)

SINP: Advanced full PhD course on Synthetic Biology (developed and teaching), basic PhD course on Biophysics and Biochemistry (teaching).

Calcutta University: M.Sc course in Medical Biotechnology B.Tech course in Reaction Engineering at Dept. Chemical Technology

Presidency Univ: MSc biostatistics, synthetic biology, and biochemical engineering, B.Sc biophysics, biochemistry and nanotechnology.

SOUMEN KANTI MANNA, PhD
Associate Professor E



RESEARCH AREAS:

Metabolomics, Lipidomics, Proteomics, Mass Spectrometry
Hepatobiliary Diseases and Cancer

EDUCATION:

2008 Ph.D. in Chemicals Sciences, TIFR, Mumbai
2002 M.Sc. in Chemistry (Inorganic), University of Calcutta
2000 B.Sc. (Hons) in Chemistry, University of Calcutta

ACADEMIC POSITIONS:

2014- Present Associate Professor 'E', Saha Institute of Nuclear Physics, Kolkata
2014 Visiting Scientist, UM-DAE CBS, Mumbai
2008-2013 Postdoctoral Fellow, National Institute of Health, USA

AWARDS/HONOURS (SELECTED):

2015 Ramanujan Fellowship, DST, India
2014 Young Investigator Award, MSACL EU-2014, Austria
2014 Young Investigator Award, MSACL-2014, USA
2013 Young Investigator Award, MSACL-2013, USA
2012 Fellows Award for Research Excellence (FARE) 2013, NIH, USA
2011 Director's Intramural Innovation Award, NCI, NIH, USA
2010 Fellows Award for Research Excellence (FARE) 2011, NIH, USA

PATENT/INNOVATIONS:

2014 International Patent Application No. PCT/US2014/012758
2013 US Patent Application No. 61/845,055
2011 US Patent Application No. 61/507,573

SELECTED PUBLICATIONS (2012-2017):

A. Research Articles

1. Patel D, Thompson M D, **Manna S K**, Krausz K W, Zhang L, Nilubol N, Gonzalez F J, Kebebew E. Unique and Novel Urinary Metabolomic Features in Malignant versus Benign Adrenal Neoplasms. *Clin Cancer Res.* 2017. PMID: 28450405
2. Golla, S., Golla, J. P. Golla, Krausz, K. W., **Manna, S. K.**, Simillion, C., Beyoglu, D., Idle, J. R., Gonzalez, F. J., Metabolomic Analysis of Mice Exposed to γ -Irradiation Reveals a Systemic Understanding of Total Body Radiation Exposure. *Radiat Res.* 2017;187(5):612-629. PMID: 28467754
3. Chen Y., Singh S., Matsumoto A., **Manna S. K.**, Abdelmegeed M. A., Golla S., Murphy R. C., Dong H, Song B. J., Gonzalez F. J., Thompson D. C., Vasiliou V. Chronic Glutathione Depletion Confers Protection against Alcohol-induced Steatosis: Implication for Redox Activation of AMP-activated Protein Kinase Pathway. *Sci Rep.* 2016;6:29743. PMID: 27403993

4. **Manna, S. K.**, Golla, S., Golla, J. P., Tanaka, N., Cai, Y., Takahashi, S., Krausz, K. W., Matsubara, T., Korboukh, I., Gonzalez, F. J., St. John's Wort Attenuates Colorectal Carcinogenesis in Mice through Suppression of Inflammatory Signaling. *Cancer Prev Res (Phila)*. 2015;8(9):786-95. PMID: 26069204
5. Mathé, E., Patterson, A. D., Majda, H., **Manna, S. K.**, Krausz, K. W., Bowman, E. D., Shields, P. G., Idle, J. R., Smith, P. B., Anami, K., Kajandjian, D. J., Hatzakis, E., Gonzalez, F. J. Harris, C. C. Non-invasive urinary metabolomic profiling identifies diagnostic and prognostic markers in lung cancer. *Cancer Res*. 2014;74(12):3259-70. PMID: 24736543
6. **Manna, S. K.**, Tanaka, T., Krausz, K. W., Majda, H., Xue, X., Matsubara, T., Bowman, E. D., Fearon, E. E., Harris, C. C., Shah, Y. M., and Gonzalez, F. J. Biomarkers of coordinate metabolic reprogramming in colorectal tumors in human and mice. *Gastroenterology* 2014;146(5):1313-24. PMID: 24440673.
7. Johnson, C. H., Manna, S. K., Krausz, K. W., Bonzo, J. A. Hollingshead, M. G., Gonzalez, F. J. Global metabolomics reveals urinary biomarkers of breast cancer in a MCF-7 Xenograft Mouse Model. *Metabolites* 2013; 3 (3); 658-672
8. **Manna, S. K.**, Krausz, K. W., Bonzo, J., Idle, J. R. and Gonzalez, F. J. Metabolomics reveals aging-associated attenuation of noninvasive radiation biomarkers in mice: potential role of polyamine catabolism and incoherent DNA damage-repair. *J Proteome Res*. 2013;12(5):2269-81. PMID: 23586774.
9. Singh, A., Happel, C., **Manna, S. K.**, Acquah-Mensah, G., Carratero, J., Kumar, S., Nasipuri, P., Krausz, K. W., Dewi, R., Wakabayashi, N., Boros, L. G., Gonzalez, F. J., Gabrielson, E., Wong, K. K., Girnun, G., Biswal, S. Nrf2 regulates miR-1 and miR-206 to drive tumorigenesis. *J Clin Invest*. 2013; 123(7): 2921–2934. PMID: 23921124
10. Bi, H, Krausz, K. W., **Manna, S. K.**, Li, F., Johnson, C. H., and Gonzalez, F. J. Optimization of harvesting, extraction and analytical protocols for UPLC-ESI-MS-based metabolomic analysis of adherent mammalian cancer cells. *Anal Bioanal Chem*. 2013;405(15):5279-89. PMID: 23604415.
11. Matsubara, T., Tanaka, T., Krausz, K. W., **Manna S. K.**, Kang, D., Anderson, E. R., Luecke, H., Patterson, A. D., Shah, Y. M., and Gonzalez, F. J. Metabolomics identifies an inflammatory cascade involved in dioxin- and diet-induced steatohepatitis. *Cell Metab*. 2012; 16(5):634-44. PMID: 23140643

B. Reviews and Book Chapters

1. **Manna, S. K.**, Thompson, M., Gonzalez, F. J. "Noninvasive biomarkers of alcoholic liver disease in mouse model" in *Biological Basis of Alcohol-Induced Cancer* (edited by Vasilis Vasiliou, Samir Zakhari, Helmut K. Seitz, Jan B. Hoek, published by Springer). *Adv Exp Med Biol*. 2015;815:217-38. PMID: 25427910

TEACHING/GUIDANCE:

- Teaching course on mass spectrometry and crystallography in University of Calcutta
- Teaching course on chromatography and mass spectrometry at SINP.
- Current Ph.D. students: 2

SUBRATA BANERJEE

Professor H



Education:

Ph.D. (Sc.), University of Calcutta, 1991;

Post M.Sc. (Bioscience), Saha Institute of Nuclear Physics (SINP), Kolkata, 1984;

M.Sc. (Physics), University of Calcutta, 1982;

B.Sc. (Physics), Presidency College, University of Calcutta, 1980;

Academic Profile:

1991-1997: Post Doctoral/Research Associate, Lineberger Cancer Centre, UNC at Chapel Hill, NC, USA;

1997-2001: Reader-'D', Biophysics Division, SINP;

2001-2005: Assoc. Prof.-'E', Biophysics Division, SINP;

2005-2010: Prof.-'F', Structural Genomics Section, SINP;

2010-2016: Prof.-'G': Biophysics & Structural Genomics Division, SINP;

2016- Present : Prof.-'H': Biophysics & Structural Genomics Division, SINP;

Honors/Award:

Fanconi's Anemia Inc. (USA) Post Doctoral Fellowship, 1992-1995;

Leukemia Society of America (LSA) Research Associate, 1995-1997;

SINP Foundation Day Lecture Award, Best Publication, 2010;

Research: Main area of interest is to understand the crosstalk between proliferation and differentiation in haemopoiesis and carcinogenesis. Currently, we are studying the role of cellular metabolism, mitochondrial dynamics, cytoskeletal signalling in cellular migration, immune evasion and aberrant differentiation – the hallmarks of cancer. Our long term goal is to design appropriate vectors for gene and stem cell therapy of haematological disorders.

Number of students supervised for Ph. D. (Sc.): 10; Number of Postdoc. (DBT) supervised: 1;

Number of students currently undergoing supervision for Ph. D. (Sc.): 2;

Other Academic/Teaching Duties: Been an Honorary Post Graduate Lecturer/ Examiner in Departments of Biotechnology, Microbiology, Neurobiology, Genetics, Calcutta University (CU), Jadavpur University (JU) and West Bengal University of Technology (WBUT); (*Subject:* Gene and Stem Cell therapy & Medical Biotechnology);

Served as a Member, Board of Studies, Department of Biotechnology, Kalyani University; Ph.D. Committee, Department of Biophysics, University of Calcutta; reviewer for various journals viz. *Blood, Leukemia, Leuk. Res., J. Biol. Chem., Virology* etc.; Reviewer research grants viz. SERB-DST, DBT, CSIR etc.;

Publications (2012-2016):

1. Pal, A.D. and Banerjee S. Epstein-Barr Virus Latent Membrane Protein 2A mediated activation of Sonic Hedgehog pathway induces HLA Class Ia downregulation in Gastric Cancer cells (2015) *Virology* **484** 22
2. Basak, N.P. and Banerjee S. Mitochondrial dependency in progression of Acute Myeloid Leukemia (2015) *Mitochondrion* **21**(3) 41
3. Roy, A and Banerjee S. p27 & Leukemia: Cell cycle and beyond (2015). *J. Cell Physiol.* **230**(3)504
4. Haldar, S., Roy, A., Banerjee S. Differential regulation of MCM7 and its intronic miRNA cluster miR-19-106b-25 during megakaryopoiesis induced polyploidy (2014) *RNA Biology* **11**(9) 1137
5. Pal, A.D., Basak, N.P., Banerjee, A.S., Banerjee, S. Epstein Barr Virus Latent Membrane Protein-2A alters mitochondrial dynamics promoting cellular migration mediated by Notch signaling pathway (2014) *Carcinogenesis* **35**(7) 1592;
6. Basak, N.P., Roy, A., Banerjee, S. Alteration of Mitochondrial Proteome due to Activation of Notch 1 Signaling Pathway (2014) *Journal of Biological Chemistry* **289**(11)7320
7. Roy, A., Haldar, S., Basak, N.P., Banerjee, S. Molecular cross talk between Notch1, Shh and Akt pathways during erythroid differentiation of K562 and HEL cell lines (2014) *Experimental Cell Research* **320**(1) 69.
8. Saha, S., Banerjee, S., Banerjee, D., Chandra, S., Chakrabarti, A. 2DGE and DIGE based proteomic study of malignant B-cells in B-cell acute lymphoblastic leukemia (2014) *EuPA Open Proteomics* **3**(6)13
9. Roy, A., Lahiry, L., Banerjee, D., Ghosh, M., Banerjee, S. Increased Cytoplasmic Localization of p27kip1 and Its Modulation of RhoA Activity during Progression of Chronic Myeloid Leukemia (2013) *PLoS ONE* **8**(10)
10. Banerjee, A.S., Pal, A.D., Banerjee, S. Epstein-Barr virus-encoded small non-coding RNAs induce cancer cell chemoresistance and migration (2013) *Virology* **443**(2) 294.
11. Roy, A., Basak, N.P., Banerjee, S. Notch1 intracellular domain increases cytoplasmic EZH2 levels during early megakaryopoiesis (2012) *Cell Death and Disease* **3**(8).



Pulak Kumar Ray, Engineer G

Head, Electron Microscopy Facility (EMF)

DOB : 24.12.1960; **E-Mail** : pulak.ray@saha.ac.in

Phone : +91-33-2337 5345 (5 lines) Extn. 3106 / 3128.

Academic Qualifications : Masters in Technology (Applied Physics), in the year 1985.

Professional qualifications : Charter Engineer, in the year 1992.

Membership of Professional bodies : Member, The Institute of Engineers.

Member, The Institution of Electronics & Telecommunication Engineers.

Employment details:

Sl. #	Organization	Period	
		From	To
1.	Sonodyne Television Co. Pvt. Ltd.	01.06.1985	04.08.1986
2.	Blue Star Ltd.	05.08.1986	10.05.1991
3.	S.I.N.P.	13.05.1991	Till date

Developmental work:

Being the Head, Electron Microscope Facility, the undersigned was entrusted to set up the complete infrastructural facility (planning and execution both) for 300keV TEM including room preparation, interior work of the room, civil work, electrical work and air-conditioning system. The state-of-the-art 300keV HRTEM equipped with STEM, EDS, EELS & HAADF (Make: FEI, Model: F30 STWIN) has been installed successfully in the year 2012. Also successfully installed the 200keV Transmission Electron Microscope (FEI, STWIN) with 0.24 nm. resolution, in the year 2006.

Achievement of the Electron Microscope Facility: The 200keV Transmission Electron Microscope (procured from the project "Structural Genomics & Biological Studies" under the mid-term appraisal of X-th five-year plan) is a Central Facility of the Institute. Its use is not limited to SINP only; it caters to the need of the interested scientists in the Eastern Region and sometimes all over India. Being the Head of the E.M. Facility, the undersigned is responsible for overall activities of the facility.

The 200keV TEM caters to the researchers from Biological Sciences and Material Sciences both. More than 30 faculty members of our Institute use the facility on regular basis. More than 20 research institutes and universities of the Eastern India along with some DAE organization (VECC, UGC-DAE etc.) also use the instrument extensively. Some of the Institutes (like: IIT-Kgp, IACS, Bose Inst., Jadavpur University, CGCRI etc.) have their own TEM but also use our facility.

Publications using the instrument More than 60 papers have been published during the period 2008 to 2015 using the instrument and the authors have duly acknowledged the Electron Microscope Facility (EMF).

National level Academic Review report

Crystallography & Molecular Biology Division

A Report for the period 2012- June 2017

Present Staff Members

Faculty Members (6)	Scientific Officers / Assistants (6)
Abhijit Chakrabarti, HoD, Senior Prof H+	Utpal Basu
Rahul Banerjee, Prof. G	Abhijit Bhattacharyya
Udayaditya Sen, Prof. G	Ashis K. Dutta
Partha Saha, Prof. G	Dr. Bikram Nath
Sampa Biswas, Prof. G	Saikat Mukherjee
H Raghuraman, Asso Prof E	Dr. Sushanta Debnath
	Tech (1) / Admin (1) / Auxiliary (2)
Faculty Members superannuated	Samir K Majumder
Prof. S Raha (November 2012)	Durga Hazra
Prof. N P Bhattacharya (January 2016)	Sakal Dev Ram
	Bipin Bose

Present Research Associate/Post doctoral fellows

Name	Year of Joining
Sumana Roy, WoS DST	September 2014
Supriya Khanra, DBT	July 2016
Chandrima Jash, SERB N-PDF	August 2016
Sanjima Pal, SINP	October 2016
Sansa Dutta, WoS DST	April 2017
Past Members	
Debi Choudhury	May 2013 – 2016
Sruti Dutta	June 2011- December 2014
Pulakesh Aich	June 2011- December 2014
Prabal K Chakraborty	November 2011 – 2013

Present Research Fellows

	Name	Year of joining	Supervisor
1	Sanghati Roychoudhury	August 2011	Udayaditya Sen
2	Kamalendu Pal	August 2012	Udayaditya Sen
3	Malti Yadav	August 2012	Udayaditya Sen
4	Shramana Chatterjee	August 2013	Udayaditya Sen
5	Benazir Alam	August 2013	Sampa Biswas
6	Dipayan Bose	August 2014	Abhijit Chakrabarti
7	Souvik Sarkar	August 2015	Abhijit Chakrabarti
8	Tulika Chakraborty	August 2015	Udayaditya Sen
9	Satyaki Chatterjee	January 2016	H Raghuraman
10	Anindita Das	August 2016	H Raghuraman
11	Gargi Biswas	August 2016	Rahul Banerjee
12	Subhoja Chakraborty	August 2016	Sampa Biswas
13	Priyadarshani Suchismita Sethy	August 2016	Partha Saha

Ph.D. Awarded

	Thesis details	Candidate	Supervisor	Present position
1	University of Calcutta, August 2012	Mithun Sinha	Nitaipada Bhattacharyya	Postdoc, Ohio State University Medical Center, USA
2	University of Calcutta, May 2013	Sudip Majumdar	Udayaditya Sen	Assistant Professor, Amity University, Gurgaon
3	Homi Bhaba National Institute, August 2013	Anup Kumar Maity	Partha Saha	School teacher
4	University of Calcutta, September 2013	Samir Das	Udayaditya Sen & Debashis Mukhopadhyay	Postdoc, University of British Columbia, Canada

5	University of Calcutta, June 2014	Sankar Basu	Rahul Banerjee	NPDF fellow, University of Delhi
6	University of Calcutta, October 2014	Kamalika Roychaudhuri	Nitaipada Bhattacharyya	Postdoc, Indian Institute of Chemical Biology, Kolkata
7	University of Calcutta, October 2014	Jayeeta Ghose	Nitaipada Bhattacharyya	Postdoc, Ohio State Univ Medical Center, USA
8	University of Calcutta, May 2015	Ramanuj Banerjee	Udayaditya Sen	Postdoc, University of Michigan, USA
9	Homi Bhaba National Institute, May 2015	Seema Nath	Udayaditya Sen	Working with NGO
10	University of Calcutta, June 2015	Kasturi Guha	Partha Saha	Not known
11	University of Calcutta, June 2015	Eashita Das	Nitaipada Bhattacharyya	Postdoc, University of Toronto, Canada
12	Homi Bhaba National Institute, July 2015	Sourav Roy	Rahul Banerjee	Postdoc, Thomas Jefferson University, USA
13	Homi Bhaba National Institute, October 2015	Barnali Waugh	Rahul Banerjee	Postdoc, Weismann Institute, Israel
14	University of Calcutta, November 2015	Srijit Das	Nitaipada Bhattacharyya	Postdoc, University of Iowa, USA
15	Homi Bhaba National Institute, May 2016	Rakhi Paul	Udayaditya Sen	Assistant professor, Bethune College, Kolkata
16	University of Calcutta, November 2016	Neha Rai	Sanghamitra Raha	Postdoc, Orebro University, Sweden
17	University of Calcutta, November 2016	Soumita Mukherjee	Partha Saha	Applied for NPDF fellowship at Bose Institute, Kolkata
	Thesis Submitted			
18	University of Calcutta, November 2016	<i>Supratim Ghatak</i>	Sanghamitra Raha	Medical writer, Pune
19	University of Calcutta June 2017	<i>Sudha Bucha</i>	Nitaipada Bhattacharyya	Not known

Major Equipments and Resources in the Division

Rotating anode X-ray generator and MAR345dtb imaging plate

Ion Proton NEXGen DNA Sequencer

Beckman Coulter Cell Lab quanta /Epics CL Flow Cytometer

Carl Zeiss Axiovert Z1 Fluorescence microscope

GE Two-dimensional gel electrophoresis system

GE Fluorescence and phosphorimager scanner (Typhoon)

Bio Tek Elisa Reader

GE ImageQuant LAS 500 Chemidoc

Varian Cary Eclipse Fluorescence Spectrophotometer

Varian Cary 50 Bio UV-Vis Spectrophotometer

Research activities

Main focus of Crystallography and Molecular Biology Division is study of the structure and conformation of proteins involved in various cellular regulatory processes. Studies relating the structure and dynamics of biological macromolecules to function are essential part of modern biophysics in order to unravel the mechanism of action of proteins at the molecular level. Our research is strongly focused on understanding the mechanistic insights of various classes of proteins such as membrane skeletal proteins; cell-cycle regulatory proteins; signaling and heat shock proteins; cysteine proteases and inhibitors; proteins involved in unique sugar metabolism; and integral membrane proteins. Using well-established expertise of recombinant DNA technology, X-ray crystallography

and structure-guided protein engineering, we attempt to understand the mechanism of proteolytic activity of cysteine proteases, alter the function of cysteine proteases (like imparting hemoglobinase activity), design and generate specific protein inhibitors from serpin family against falcipain2 from *Plasmodium falciparum*, a drug target for the malaria parasite. Structural and functional aspects of *Vibrio cholera* proteins involved in many processes such as c-di-GMP mediated biofilm formation, transcription termination and activation (Rho-specific), small heat shock proteins (HSP31, HSP15, DnaK etc.) mediated protein folding and protein phosphorylation / dephosphorylation involved in metabolic activity and signal transduction will be studied in great detail.

Several unique sugar metabolizing proteins have been identified in *Leishmania donovani*, a protozoan parasite that causes Leishmaniasis, which are potential drug targets. Structural characterizations have been initiated with the proteins UDP-Glc 4'-epimerase, UDP-galactopyranose mutase and Galactose Mutarotase. Works are in progress to elucidate the functional interaction of DNA repair protein (Ku) with the cell cycle modifier polo-like kinase 1 (Plk1). Further, structural and thermodynamic insights related to the interaction of cyclophilin, a peptidyl-prolyl cis-trans isomerase, with a transmembrane protein CD147 would be examined since this interaction has been implicated in inflammation, cancer and cardiac disorders. We would use the newly installed Next Generation Sequencer (NGS) to elucidate any differential relationship of involvement of Ku with the origin-uses in a spatio-temporal manner. Another line of research would focus on the altered drug resistance in *Leishmania* strains against available drugs. NGS would effectively be used to identify proteins/pathways involved in drug resistance.

Erythroid spectrin is a major constituent of Red Blood Cells (RBC) and plays a vital role in maintaining the cytoskeletal structure and flexibility of the erythrocyte. Cloning, expression and purifications of spectrin domains such as the ankyrin binding domain, self-associating domain, SH3 domains etc have been initiated to explore their protein-protein interactions, chaperone activity and membrane

binding potential. We are starting a new research area on characterizing the structural dynamics of membrane proteins. Importantly, ~30% of human genome codes for membrane proteins and ~60% of available drugs target membrane proteins. Structural dynamics of potassium and magnesium ion channels have been just initiated to decipher lipid-dependent voltage gating mechanisms.

Important Results

- Structural biology of cyclophilin, cysteine proteases, *Vibrio cholera* proteins, sugar metabolizing proteins and protein inhibitors from serpin family, important target for malaria, Leishmania and biofilm formation has been done.
- Next Generation Sequencer (NGS) installed and standardized to effectively use to identify proteins/pathways involved in drug resistance.
- Cloning, expression and purifications of spectrin domains such as the ankyrin binding domain, self-associating domain, SH3 domains etc have been initiated to explore potential for acting as alternative target of anticancer drugs.
- New research area on characterization and studying the structural, function, dynamics of membrane proteins has been initiated.
- 17 PhD awarded and 84 publications made in peer-reviewed journals of international repute.

Future Research Plans

Our research is strongly focused on understanding the mechanistic insights of various classes of proteins at the molecular level that are crucial in important cellular processes such as ion transport and excitability, maintaining cellular architecture, biofilm formation, DNA replication, proteolysis, sugar metabolism etc. These proteins include cytoskeletal proteins, cell-cycle regulatory proteins, signaling and heat shock proteins, cysteine proteases and inhibitors, proteins

involved in unique sugar metabolism, and integral membrane proteins that are involved in ion transport mechanisms.

Using our well-established expertise in recombinant DNA technology, X-ray crystallography and structure-guided protein engineering, we will attempt to understand the mechanism of proteolytic activity of cysteine proteases, alter the function of cysteine proteases (like imparting hemoglobinase activity), design and generate specific protein inhibitors from serpin family against falcipain2 from *Plasmodium falciparum*, a drug target for the malaria parasite. Structural and functional aspects of *Vibrio cholera* proteins involved in many processes such as c-di-GMP mediated biofilm formation, transcription termination and activation (Rho-specific), small heat shock proteins (HSP31, HSP15, DnaK etc.) mediated protein folding and protein phosphorylation/dephosphorylation involved in metabolic activity and signal transduction will be studied in great detail. Functional interaction of DNA repair protein (Ku) with the cell cycle modifier polo-like kinase 1 (Plk1) will be monitored, and the Next Generation Sequencer will be used to elucidate any differential relationship of involvement of Ku with the origin-uses in a spatio-temporal manner. Several unique sugar metabolizing proteins have been identified in *Leishmania donovani*, which is a protozoan parasite and causes Leishmaniasis, and are potential drug targets. These proteins (UDP-Glc 4'-epimerase, UDP-galactopyranose mutase, Galactose Mutarotase etc.) will be targeted for structure determination. Further, structural and thermodynamic insights related to the interaction of cyclophilin, a peptidyl-prolyl cis-trans isomerase, with a transmembrane protein CD147 will be examined since this interaction has been implicated in inflammation, cancer and cardiac disorders. The role of Erythroid 'spectrin repeat' domains in chaperone activity, membrane binding potential, protein-protein interactions will be explored.

Recently, we have started a new research area on characterizing the structural dynamics of membrane proteins. Site-directed spin labeling (SDSL) and Electron Paramagnetic Resonance (EPR) spectroscopy is a powerful technique to provide structural and dynamic information on protein function. Importantly, low-resolution models of proteins in different functional states can be obtained which

are not amenable to crystallographic approaches. We would like to establish this facility in SINP. Regarding the structural dynamics of membrane proteins, research will be focused on understanding the activation gating mechanisms of potassium and magnesium ion channels, and lipid-dependent gating mechanisms. We will establish Electron Paramagnetic Resonance (EPR) spectroscopy as a major central facility in the Division.

List of publications in peer-reviewed Journals

Publications during 2012

1. Choudhury KR, Raychaudhuri S, Bhattacharyya NP (2012) Identification of HYPK-Interacting Proteins Reveals Involvement of HYPK in Regulating Cell Growth, Cell Cycle, Unfolded Protein Response and Cell Death, *PLoS One*. 7(12): e51415.
DOI: 10.1371/journal.pone.0051415.
2. Bhattacharjya S, Nath S, Ghose J, Maiti GP, Biswas N, Bandyopadhyay S, Panda CK, Bhattacharyya NP, Roychoudhury S (2013) miR-125b promotes cell death by targeting spindle assembly checkpoint gene MAD1 and modulating mitotic progression, *Cell Death Differ*. 20, 430-442
DOI: 10.1038/cdd.2012.135
3. Sinha M, Mukhopadhyay S, Bhattacharyya NP (2012) Mechanism(s) of alteration of micro RNA expressions in Huntington's disease and their possible contributions to the observed cellular and molecular dysfunctions in the disease, *Neuromolecular Med*. 14(4):221-43.
DOI: 10.1007/s12017-012-8183-0
4. Paul R, Nath S, Sen U (2012) Cloning, expression, purification, crystallization and preliminary X-ray analysis of a fructokinase from *Vibrio cholerae* O395, *Acta Crystallogr. Sect. F Struct. Biol. Cryst. Commun*. 68(12):1564-7.
DOI: 10.1107/S1744309112047598.
5. Banerjee R, Nath S, Ranjan A, Khamrui S, Pani B, Sen R, Sen U (2012) The first structure of polarity suppression protein, psu from enterobacteria phage p4, reveals a novel fold and a knotted dimer, *J. Biol. Chem*. 287(53):44667-75.
DOI: 10.1074/jbc.M112.423202
6. Nath S, Banerjee R, Khamrui S, Sen U (2012) Cloning, purification, crystallization and preliminary X-ray analysis of two low-molecular-weight protein tyrosine phosphatases from *Vibrio cholerae*, *Acta Crystallogr. Sect. F Struct. Biol. Cryst. Commun*. 68(10):1204-8.
DOI: 10.1107/S174430911203518X.

7. Majumder S, Khamrui S, Dasgupta J, Dattagupta JK, Sen U (2012) Role of remote scaffolding residues in the inhibitory loop pre-organization, flexibility, rigidification and enzyme inhibition of serine protease inhibitors, *Biochim. Biophys. Acta.* 2012 Jul;1824(7): 882-90.
DOI: 10.1016/j.bbapap.2012.04.009.
8. Maity AK, Saha P. (2012) The histone acetyl transferase LdHAT1 from *Leishmania donovani* is regulated by S-phase cell cycle kinase. *FEMS Microbiol. Lett.* 336(1): 57-63.
DOI: 10.1111/j.1574-6968.2012.02656.x.
9. Basu S, Bhattacharyya D, Banerjee R (2012) Self-complementarity within proteins: bridging the gap between binding and folding, *Biophys. J.* 102(11): 2605-14.
DOI: 10.1016/j.bpj.2012.04.029
10. Roy S, Choudhury D, Aich P, Dattagupta JK, Biswas S (2012) The structure of a thermostable mutant of pro-papain reveals its activation mechanism, *Acta Crystallogr. D Biol. Crystallogr.* 68(12): 1591-603.
DOI: 10.1107/S0907444912038607
11. Roy S, Dattagupta JK, Biswas S (2012) Expression of recombinant human cathepsin K is enhanced by codon optimization, *Process Biochem.* 47, 1944–1947.
DOI: 10.1016/j.procbio.2012.06.029
12. Khanra S, Datta S, Mondal D, Saha P, Bandopadhyay SK, Roy S, Manna, M (2012) RFLPs of ITS, ITS1 and hsp70 amplicons and sequencing of ITS1 of recent clinical isolates of Kala-azar from India and Bangladesh confirms the association of *L. tropica* with the disease. *ActaTropica* 124: 229– 234
DOI: 10.1016/j.actatropica.2012.08.017

Publications during 2013

1. Das E, Jana NR, Bhattacharyya NP (2013) MicroRNA-124 targets CCNA2 and regulates cell cycle in STHdh^(Q111)/Hdh^(Q111) cells, *Biochem Biophys Res Commun.*,437, 217-224
DOI: 10.1016/j.bbrc.2013.06.041
2. Basu M, Bhattacharyya NP, Mohanty PK (2013) Comparison of modules of wild type and mutant Huntingtin and TP53 protein interaction networks: implications in biological processes and functions, *PLoS One.* 8(5):e64838
DOI: 10.1371/journal.pone.0064838
3. Goswami A, Banerjee R, Raha S (2013) Drought resistance in rice seedlings conferred by seed priming : role of the anti-oxidant defense mechanisms, *Protoplasma* 250(5): 1115-29
DOI: 10.1007/s00709-013-0487-x

4. Ranjan A, Banerjee R, Pani B, Sen U, Sen R (2013) The moonlighting function of bacteriophage P4 capsid protein, Psu, as a transcription antiterminator, *Bacteriophage*. 3(2):e25657 .
DOI: 10.4161/bact.25657
5. Biswas M, Dey S, Khamrui S, Sen U, Dasgupta J (2013) Conformational Barrier of CheY3 and Inability of CheY4 to Bind FlIM Control the Flagellar Motor Action in *Vibrio cholera*, *PLoS One*. 8(9):e73923
DOI: 10.1371/journal.pone.0073923
6. Nath S, Banerjee R, Sen U (2013) A Novel 8-nm Protein Cage Formed by *Vibrio cholerae* Acylphosphatase, *J. Mol. Biol.* 426(1), 36-38
DOI: 10.1016/j.jmb.2013.09.014
7. Ranjan A, Sharma S, Banerjee R, Sen U, Sen R (2013) Structural and mechanistic basis of anti-termination of Rho-dependent transcription termination by bacteriophage P4 capsid protein Psu, *Nucleic Acids Res.* 41(14):6839-56
DOI: 10.1093/nar/gkt336
8. Dutta S, Dattagupta JK, Biswas S (2013) Enhancement of proteolytic activity of a thermostable papain-like protease by structure-based rational design, *PLoS One*. 8(5):e62619
DOI: 10.1371/journal.pone.0062619
9. Mitra P, Banerjee M, Biswas S, Basu S (2013) Protein interactions of Merocyanine 540: spectroscopic and crystallographic studies with lysozyme as a model protein, *J. Photochem. Photobiol. B*. 121:46-56
DOI: 10.1016/j.jphotobiol.2013.02.010
10. Goswami S, Sen D, Das AK, Das NK, Aich K, Fun HK, Quah CK, Maity AK, Saha P (2013) A new rhodamine-coumarin Cu²⁺ –selective colorimetric and ‘off–on’ fluorescence probe for effective use in chemistry and bioimaging along with its bound X–ray crystal structure, *Sensor Actuat: B Chem.* 183, 518-15
DOI: 10.1016/j.snb.2013.04.005
11. Goswami S, Das AK, Maity AK, Manna A, Aich K, Maity S, Saha P , Mandal TK (2013) Visual and near IR (NIR) fluorescence detection of Cr³⁺ in aqueous media via spirobenzopyran ring opening with application in logic gate and bio-imaging, *Dalton Trans.* 43, 231-39
DOI: 10.1039/C3DT51851E
12. Goswami S, Manna A, Maity AK, Paul S, Das AK, Das MK, Saha P, Quah CK, Fun HK (2013) Selective detection and bio-imaging of Pd²⁺ with novel ‘C–CN’ bond cleavage of cyano-hodamine, cyanation with diaminomaleonitrile, *Dalton Trans* 42, 12844 – 48
DOI: 10.1039/C3DT51591E

Publications during 2014

1. Guha K, Bhandari D, Sen T, Saha P (2014) Ubiquitination mediated interaction among domains is responsible for inhibition of RNA endonuclease activity of mRNA cycling sequence binding protein from *L. donovani* (LdCSBP). *Parasitol. Res.* 113(8), 2941–49
DOI: 10.1007/s00436-014-3956-z
2. Ghosh S, Chakraborty P, Saha P, Acharya S, Ray M (2014) Polymer based Nanoformulation of Methylglyoxal as an Antimicrobial Agent: Efficacy against Resistant Bacteria, *RSC Adv.* 4, 23251-61
DOI: 10.1039/C4RA00075G
3. Banerjee S, Chaudhuri S, Maity AK, Saha P, Pal SK (2014) Role of Caffeine in DNA Recognition of a Potential Food-Carcinogen Benzo[a]pyrene and UVA induced DNA damage, *J. Molecular Recognition*, 27(8) 510-20
DOI: 10.1002/jmr.2379
4. Koley Seth B, Ray A, Saha A, Saha P, Basu S (2014) Potency of photoinduced electron transfer and antioxidant efficacy of pyrrole and pyridine based Cu(II)-Schiff complexes while binding with CT-DNA. *J Photochem. Photobiol. B: Biology* 132, 72-84
DOI: 10.1016/j.jphotobiol.2014.02.007
5. Koley Seth B, Ray A, Biswas S, Basu S (2014) Ni(II) - Schiff base complex as enzyme inhibitor of hen egg white lysozyme: a crystallographic and spectroscopic study. *Metallomics*, 6, 1737-47
DOI: 10.1039/C4MT00098F
6. Roy S, Basu S, Datta AK, Bhattacharyya D, Banerjee R, Dasgupta D (2014) Equilibrium unfolding of cyclophilin from *Leishmania donovani* : Characterization of intermediate states. *Inter. J. Biol. Macromol.* 69: 353-360
DOI: j.ijbiomac.2014.05.063
7. Basu S, Bhattacharyya D, Banerjee R (2014) Applications of the complementarity plot in error detection and structure validation of proteins. *Ind. J. Biochem. Biophys.* 51: 188-200
<http://nopr.niscair.res.in/handle/123456789/29083>
8. Nath S, Banerjee R, Sen U. (2014) Atomic resolution crystal structure of VcLMWPTP-1 from *Vibrio cholerae*O395: Insights into a novel mode of dimerization in the low molecular weight protein tyrosine phosphatase family. *Biochem Biophys Res Commun.* 450(1) 390–95
DOI:10.1016/j.bbrc.2014.05.129.
9. Waugh B, Ghosh A, Bhattacharya D, Ghoshal N, Banerjee R (2014) In silico work flow for scaffold hopping in leishmania. *BMC Res. Notes*, 7: 802
DOI: 10.1186/1756-0500-7-802

10. Guha K, Das S, Saha P (2014) Lys-413 of S-phase mRNA cycling sequence binding protein from *Leishmania donovani* (LdCSBP) is modified through monoubiquitination that is responsible for inhibition of its ribonuclease activity. *Ind. J. Biochem. Biophys.* 51, 559-566.
http://nopr.niscair.res.in/handle/123456789/30507
11. Raychaudhuri S, Banerjee R, Mukhopadhyay S, Bhattacharyya NP (2014) Conserved C-terminal nascent peptide binding domain of HYPK facilitates its chaperone-like activity. *J Biosci.* 39(4), 659-72.
DOI: 10.1007/s12038-014-9442-z
12. Das S, Bhattacharyya NP (2014) Heat shock factor 1 regulates hsa-miR-432 expression in human cervical cancer cell line. *Biochem. Biophys. Res. Commun.* 453(3), 461-6.
DOI: 10.1016/j.bbrc.2014.09.100.
13. Bag AK, Saha S, Sundar S, Saha B, Chakrabarti A, Mandal C (2014) Comparative proteomics and glycoproteomics of plasma proteins in Indian visceral leishmaniasis. *Proteome Sci.* 12: 48
DOI:10.1186/s12953-014-0048-z

Publications during 2015

1. Das A, Chakrabarti A, Das PK (2015) Suppression of protein aggregation by gold nanoparticles : A new way to store and transport proteins. *RSC Adv.* 5, 38558 – 70
DOI: 10.1039/C4RA17026A
2. Chakrabarti A, Patra M (2015) Differential interactions of two local anesthetics with phospholipid membrane and nonerythroid spectrin: localization in presence of cholesterol and ganglioside, GM1. *BBA – Biomembr.* 1848, 821-832.
DOI: 10.1016/j.bbamem.2014.11.022
3. Basu A, Chakrabarti A (2015) Defects in erythrocyte membrane skeletal Architecture. *Adv. Exp. Med. Biol.*, 842, 41-59
DOI: 10.1007/978-3-319-11280-0_4
4. Patra M, Mukhopadhyay C, Chakrabarti A (2015) Probing conformational stability and dynamics of erythroid and nonerythroid spectrin: Effects of urea and guanidine hydrochloride. *PLoS One* 10(1), e0116991
DOI: 10.1371/journal.pone.0116991
5. Chaudhuri S, Sardar S, Bagchi D, Dutta S, Debnath, Saha P, Lemmens P, Pal SK (2016) Photoinduced Dynamics and Toxicity of a Cancer Drug in Proximity of Inorganic Nanoparticles under Visible Light, *ChemPhysChem* 17(2) 270–77
DOI: 10.1002/cphc.201500905

6. Dey S, Biswas M, Sen U, Dasgupta J (2015) Unique ATPase site architecture triggers cis-mediated synchronized ATP binding in heptameric AAA+ ATPase domain of flagellar regulatory protein FlrC. *J. Biol. Chem.*, 290(14), 8734-47
DOI: 10.1074/jbc.M114.611434
7. Majumder S, Khamrui S, Banerjee R, Bhowmik P, Sen U (2015) A conserved tryptophan (W91) at the barrel-lid junction modulates the packing and stability of Kunitz (STI) family of inhibitors. *Biochim. Biophys. Acta.* 1854(1), 55-64
DOI: 10.1016/j.bbapap.2014.10.021
8. Paul R, Patra MD, Sen U (2015) Crystal structure of apo and ligand bound Vibrio cholerae ribokinase (Vc-RK): role of monovalent cation induced activation and structural flexibility in sugar phosphorylation. *Adv. Exp. Med. Biol.* 842, 293-307
DOI: 10.1007/978-3-319-11280-0_19
9. Choudhury KR, Bhattacharyya NP (2015) Chaperone protein HYPK interacts with the first 17 amino acid region of Huntingtin and modulates mutant HTT-mediated aggregation and cytotoxicity. *Biochem. Biophys. Res. Commun.*, 456(1),66-73.
DOI: 10.1016/j.bbrc.2014.11.035.
10. Ghatak SK, Majumdar D, Singha A, Sen S, Das D, Chakrabarti A, Mukhopadhyay C, Sen K (2015) Peanut Protein Sensitivity Towards Trace Iron : A Novel Mode to Ebb Allergic Response, *Food Chem.*, 176, 308–313.
DOI: 10.1016/j.foodchem.2014.12.081
11. Das S, Bhattacharyya NP (2015) Widening HSF1 horizon: the microRNA connection. *RNA & Disease* 2:e596.
DOI: 10.14800/rd.596.
12. Ghose J, Bhattacharyya NP, (2015) Transcriptional regulation of microRNA-100, -146a, and -150 genes by p53 and NFκB p65/RelA in mouse striatal STHdh^(Q7) / Hdh^(Q7) cells and human cervical carcinoma HeLa cells. *RNA Biol.* 2015; 12(4), 457-77.
DOI: 10.1080/15476286.2015.1014288.
13. Patra M, Mukhopadhyay, Chakrabarti A (2015) Malachite green interacts with the membrane skeletal protein, Spectrin. *RSC Adv.* 5, 91166 –76
DOI: 10.1039/C5RA15488J
14. Bucha S, Mukhopadhyay D, Bhattacharyya NP (2015) Regulation of mitochondrial morphology and cell cycle by microRNA-214 targeting Mitofusin2. *Biochem. Biophys. Res. Commun.* 465(4), 797-802.
DOI: 10.1016/j.bbrc.2015.08.090.
15. Choudhury KR, Bucha S, Baksi S, Mukhopadhyay D, Bhattacharyya NP. (2016) Chaperone-like protein HYPK and its interacting partners augment autophagy. *Eur J Cell Biol.* 95(6-7), 182-94.

DOI: 10.1016/j.ejcb.2016.03.003.

16. Rai N, Sarkar M, Raha S (2015) Piroxicam, a traditional non-steroidal anti-inflammatory drug (NSAID) causes apoptosis by ROS mediated Akt activation. *Pharmacol Rep.* 67(6),1215-23.
DOI: 10.1016/j.pharep.2015.05.012
17. Ghatak S, Raha S (2015) Micro RNA-214 contributes to proteasome independent downregulation of beta catenin in Huntington's disease knock-in striatal cell model STHdhQ111/Q111. *Biochem. Biophys. Res. Commun.* 459 (3): 509-14
DOI: 10.1016/j.bbrc.2015.02.137
18. Ray M, Rai N, Jana K, Ghatak S, Basu A, Mustafi SB, Raha S (2015) Beta catenin is degraded by both caspase-3 and proteasomal activity during resveratrol-induced apoptosis in HeLa cells in a GSK3 beta-independent manner. *Ind. J. Biochem. Biophys.* 52(1), 7-13
<http://nopr.niscair.res.in/handle/123456789/31258>
19. Ghorai A, Sarma A, Bhattacharyya NP, Ghosh U (2015) Carbon ion beam triggers both caspase-dependent and caspase-independent pathway of apoptosis in HeLa and status of PARP-1 controls intensity of apoptosis, *Apoptosis*, 20 (4), 562-80
DOI: 10.1007/s10495-015-1107-3
20. Roy S, Basu S, Dasgupta D, Bhattacharyya D, Banerjee R. (2015). The Unfolding MD Simulations of Cyclophilin: Analyzed by Surface Contact Networks and Their Associated Metrics. *PLoS One* 10: e0142173
DOI: 10.1371/journal.pone.0142173
21. Basu A, Chakrabarti A (2015) Haemoglobin Interacting Proteins and Implications of Spectrin Haemoglobin Interaction. *J Proteomics*, 128, 469 – 475
DOI: 10.1016/j.jprot.2015.06.014
22. Basu A, Speicher K, Sriswasdi S, Harper S, Pesciotta E, Chakrabarti A, Speicher DW (2015) Unexpected Red Cell Membrane Skeletal Components and Interactions. *J. Proteomics* 128, 298 – 305.

Publications during 2016

1. Choudhury KR, Das S, Bhattacharyya NP. (2016) Differential proteomic and genomic profiling of mouse striatal cell model of Huntington's disease and control; probable implications to the disease biology *J Proteomics* 132, 155 – 166
DOI: 10.1016/j.jprot.2015.11.007
2. Das D, Pramanik U, Patra M, Banerjee M, Chakrabarti A (2016) Differential interactions of imatinib mesylate with the membrane skeletal protein, spectrin and hemoglobin. *RSC Advance.* 6, 55203 – 10.
DOI: 10.1039/C5RA27276A

3. Dutta S, Choudhury D, Roy S, Dattagupta JK, Biswas S (2016) Mutation in the pro-peptide region of a cysteine protease leads to altered activity and specificity - A structural and biochemical approach. *PLoS One* 11(6): e0158024
DOI: 10.1371/journal.pone.0158024
4. Choudhury KR, Bucha S, Baksi S, Mukhopadhyay D, Bhattacharyya NP. (2016) Chaperone-like protein HYPK and its interacting partners augment autophagy. *Eur J Cell Biol.* 95(6-7) 182-94
DOI: 10.1016/j.ejcb.2016.03.003
5. Das S, Bhattacharyya NP. (2016) Huntingtin interacting protein HYPK is a negative regulator of heat shock response and is downregulated in models of Huntington's Disease. *Exp Cell Res.* May 1; 343: 107-117.
DOI: 10.1016/j.yexcr.2016.03.021
6. Kumari C, Sain D, Kumar A, Debnath S, Saha P, Dey S (2016) A real time colorimetric 'two in one' kit for tracking ppb levels of uric acid and Hg²⁺ in live HeLa S3 cells and Hg²⁺ induced keto-enol tautomerism, *RSC Adv.* 6(67):62990 – 98
DOI: 10.1039/C6RA06987H
7. Ganguly BN, Verma V, Chatterjee D, Satpati B, Debnath S, Saha P (2016) Study of Gallium Oxide Nanoparticles Conjugated with β -Cyclodextrin: An Application to Combat Cancer, *ACS Appl. Mater. Interf.* 8(27)
DOI: 10.1021/acsami.6b04807
8. Waugh B, Sen U, Banerjee R (2016) Crystal structure of phosphoglucomutase from *Leishmania major* at 3.5 angstrom resolution. *Biochemie*, 121, 102 – 11.
DOI: 10.1016/j.biochi.2015.11.015
9. Das A, Chakrabarti A, Das PK (2016) Probing protein adsorption on nanoparticle surface by second harmonic light scattering. *Phys Chem Chem Phys.* 18: 24325 – 31.
DOI: 10.1039/C6CP02196D
10. Mukherjee S, Chakraborty P, Saha P (2016) Phosphorylation of Ku70 subunit by cell cycle kinases modulates the replication related function of Ku heterodimer. *Nucleic Acids Res.* 44: 7755-65
DOI: 10.1093/nar/gkw622
11. Kratochvil HT, Carr JK, Matulef K., Annen AW, Li H, Maj M, Ostmeyer J, Serrano AL, Raghuraman H, Moran SD, Skinner JL, Perozo E, Roux B, Valiyaveetil FI., Zanni MT (2016) Instantaneous ion configurations in the K⁺ ion channel selectivity filter revealed by 2D IR spectroscopy. *Science* 353: 1040-44.
DOI: 10.1126/science.aag1447

12. Parashar K, Ballav N, Debnath S, Pillay K, Maity A (2016) Hydrous TiO₂@ polypyrrole hybrid nanocomposite as an efficient selective scavenger for the defluoridation of drinking water, *RSC Adv*, 6(101): 99482-95
DOI: 10.1039/C6RA20151B
13. Kanrar S, Debnath S, De P, Parashar K, Pillay K, Sasikumar P, Ghosh UC (2016) Preparation, characterization and evaluation of fluoride adsorption efficiency from water of iron-aluminium oxide-graphene oxide composite material, *Chem Eng. J* 306: 269-79
DOI: 10.1016/j.cej.2016.07.037
14. Parashar K, Ballav N, Debnath S, Pillay K, Maity A (2016) Rapid and efficient removal of fluoride ions from aqueous solution using a polypyrrole coated hydrous tin oxide nanocomposite, *J. Colloid Interf. Sci.* 476, 103-118
DOI: 10.1016/j.jcis.2016.05.013
15. Chatterjee T, Halder S, Chakravarty S, Chakravarty A, *Chakrabarti A* (2016) A FACS based case study on two HbE- β thalassaemia member of a family, having similar mutational background, *Scientifica* 3181937.
DOI: 10.1155/2016/3181937

Publications during 2017 (Upto 30th June)

1. Patra M, Mandal M, Chakrabarti A, Mukhopadhyay C (2017) Localization and dynamics of the anticarcinogenic Curcumin with GM1 and other micellar assemblies. *Glycoconjugate J.* 34: 171 – 179.
DOI:10.1007/s10719-016-9748-1
2. Das S, Roy Chowdhury S, Dey S, Sen U (2017) Structural and biochemical studies on *Vibrio cholerae* Hsp31 reveals a novel dimeric form and Glutathione-independent Glyoxalase activity. *PLoS ONE* 12(2): e0172629.
DOI: 10.1371/journal.pone.0172629
3. Das A, Chakrabarti A, Das PK (2017) Enzyme adsorption on nanoparticle surface probed by highly sensitive second harmonic light scattering. *Methods Enzymol.* (2017) 590, 33 – 58.
DOI: 10.1016/bs.mie.2017.01.020
4. Bose D, Patra M, Chakrabarti A (2017) Effect of pH on conformational stability, oligomerization and dynamics of erythroid and nonerythroid spectrin. *BBA Proteins & Proteomics.* 1865, 694 – 702.
DOI: 10.1016/j.bbapap.2017.03.012.
5. Giri R, Chakrabarti A, Mukhopadhyay M. (2017) Cholesterol Induced Structural Changes in Saturated Phospholipid Model Membranes Revealed Through X-Ray Scattering Technique. *J Phys Chem B.* 121, 4081 – 4090.
DOI: 10.1021/acs.jpcc.6b12587

6. Karmakar S, Banerjee D, Chakrabarti A (2017) Platelet proteomics in chronic myelogenous leukemia, *Int. J. Blood Disorders Diseases*. 1, 1-6
7. Kumari C, Sain D, Kumar A, Debnath S, Saha P, Dey S (2017) Intracellular detection of hazardous Cd²⁺ through a fluorescence imaging technique by using a nontoxic coumarin based sensor, *Dalton Trans.* 46, 2524-2531
DOI:10.1039/C6DT04833A
8. Kumari C, Sain D, Kumar A, Nayek HP, Debnath S, Saha P, Dey S (2017) A bis-hydrazone derivative of 2, 5-furandicarboxaldehyde with perfect hetero-atomic cavity for selective sensing of Hg (II) and its intracellular detection in living HeLa S3 cell, *Sensor Actuat. B: Chem.* 243, 1181-1190
DOI: 10.1016/j.snb.2016.12.103
9. Debnath S, Ballav N, Maity A, Pillay K (2017) Competitive adsorption of ternary dye mixture using pine cone powder modified with β -cyclodextrin, *J. Mol. Liq.* 225, 679-688
DOI: 10.1016/j.molliq.2016.10.109
10. Debnath S, Chakrabarti A, Nath B (2017) Flow Cytometric Analysis of Protein Aggregates, *Protein Pept. Lett.* (In Press)

Books :

Biochemical Roles of Eukaryotic Cell Surface Macromolecules, in *Advances in Experimental Medicine & Biology*, A. Chakrabarti, A. Surolia (eds.), Springer International Publishing Switzerland 2015.

Indian Philosophy and Meditation: Perspectives on consciousness. Banerjee R and Chatterjee A, Routledge, Taylor and Francis Group Publication, 2017

Faculty Members of C & MB Division :



Abhijit Chakrabarti

PhD, Indian Institute of Science, Bengaluru

Positions held (in chronological order)

Year (s)	University / Institution	Positions
2012 - 2016	Homi Bhabha National Institute	Professor H
July 2016 till date	Homi Bhabha National Institute	Senior Prof, H+
January 2014	Crystallography & Molecular Biology	HOD
April 2010 – June 2014	Centre for Advanced Research & Education	Head
Jan 2014 – Dec 2016	The Proteomics Society – India	Vice President
Sept 2011 – 2014	National Institute of Technology, Durgapur	Member, BOG
Sept 2009 – Feb 2015	National Institute of Technology, Durgapur	Senate Member
Oct 2012 – Nov 2015	West Bengal State Council of Higher Education	
Oct 2011 till date	Governing Body of the West Bengal State Council of Biotechnol	
Nov 2015 till date	Dean-Academic (Biological & Chemical Sciences), HBNI	
July 2015 till date	Member, Board of Studies (Life Science), HBNI	
April 2016 till date	Member, Executive Council of Kalyani University	
December 2016	Member, Internal Quality Assurance Cell (IQAC) of HBNI	

Research Interests :

Membrane Skeleton (Transbilayer asymmetry of aminophospholipids, PE and PS, spectrin-based network, spectrin & its recombinant constructs, hydrophobic ligand binding, chaperone-activity, interaction with hemoglobin variants, globin chains, implications in hemoglobinopathy) *Red cell and Platelet proteomics in haematological diseases* e.g. sickle cell disease and thalassemia using 2DGE and MALDI ToF/ToF mass spectrometry.

Currently working on recombinant spectrin constructs to identify the structural origin and substrate specificity of the molecular chaperone function of spectrin, phospholipid interactions and studying the potential of the actin binding anti-cancer drugs for the major membrane skeletal protein, spectrin.

Also, initiated work on characterization of different types of protein aggregates and study of protein stability using metal nanoparticle formulations.

Altogether, published thirty six (36) papers during January 2012 till June 2017 and have supervised seven (7) theses for PhD. The average impact factor of all 36 papers is 2.6 with about 160 total citations.

List of few recent publications :

1. S. Debnath, A Chakrabarti, B Nath (2017) Flow Cytometric Analysis of Protein Aggregates, Protein Pept. Lett. (*in press*)
2. R Giri, A Chakrabarti & M Mukhopadhyay. (2017) Cholesterol Induced Structural Changes in Saturated Phospholipid Model Membranes Revealed Through X-Ray Scattering Technique. J Phys Chem B. **121**, 4081 – 4090.
3. D Bose, M Patra & A Chakrabarti. (2017) Effect of pH on conformational stability, oligomerization and dynamics of erythroid and nonerythroid spectrin. (2017) BBA Proteins & Proteomics. **1865**, 694 – 702.
4. A Das, A Chakrabarti & P K Das. (2017) Enzyme adsorption on nanoparticle surface probed by highly sensitive second harmonic light scattering. Methods Enzymol. (2017) **590**, 33 – 58.
5. A Das, A Chakrabarti & PK Das. (2016) Probing protein adsorption on nanoparticle surface by second harmonic light scattering. Phys Chem Chem Phys. **18**, 24325 – 24331.
6. D Das, U Pramanik, M Patra, M Banerjee & A Chakrabarti. (2016) Differential interactions of imatinib mesylate with the membrane skeletal protein, spectrin and hemoglobin. RSC Advance **6**, 55203 – 55210.
7. A Chakrabarti, S Halder & S Karmakar. (2016). Erythrocyte & Platelet Proteomics in Haematological Disorders. Proteomics Clin Appl. **10**, 403-414.
8. S Karmakar, D Banerjee & A Chakrabarti. (2016). Platelet proteomics in thalassemia. Factors responsible for hyperquagulation. Proteomics Clin Appl. **10**, 239-247.
9. M Mitra, M Patra & A Chakrabarti. (2015). Fluorescence study of the effect of cholesterol on spectrin-aminophospholipid interactions. Eur Biophys J. **44**, 635 – 645.
10. A Basu & A Chakrabarti. (2015). Haemoglobin Interacting Proteins and Implications of Spectrin Haemoglobin Interaction. J Proteomics **128**, 469 – 475.
11. S Halder, RK Dey, A Roy Chowdhury, P Bhattacharya & A Chakrabarti. (2015) Differential regulation of urine proteins in urothelial neoplasm. J Proteomics **127**, 185 – 192.
12. A Das, A Chakrabarti & PK Das. (2015) Suppression of protein aggregation by gold nanoparticles : A new way to store and transport proteins. RSC Advances. **5**, 38558 – 38570.
13. M Patra, C Mukhopadhyay & A Chakrabarti. (2015). Probing conformational stability and dynamics of erythroid and nonerythroid spectrin : Effects of urea and guanidine hydrochloride. PLoS One **10(1)**, e0116991.
14. A Chakrabarti and M Patra. (2015). Differential interactions of two local anesthetics with phospholipid membrane and nonerythroid spectrin : localization in presence of cholesterol and ganglioside, GM₁. Biochim Biophys Acta **1848**, 821-832.
15. A Chakrabarti, D Bhattacharya, S Deb & M Chakraborty. (2013) Differential thermal stability and oxidative vulnerability of the hemoglobin variants, HbA₂ and HbE. PLOS ONE **8(11)**, e81820.
16. A Basu, S Saha, S Karmakar, S Chakravarty, D Banerjee, BP Dash & A Chakrabarti. (2013) 2D DIGE based proteomics study of erythrocyte cytosol in sickle cell disease : altered proteostasis & oxidative stress. Proteomics **13**, 3233-3242.
17. M Banerjee, A Chakrabarti & S Basu. (2012). Oxidative interaction between oxyHb and ATP : A Spectroscopic Study. J Phys Chem B. **116**, 6150-6157.

Biochemical Roles of Eukaryotic Cell Surface Macromolecules, in *Advances in Experimental Medicine & Biology*, A. Chakrabarti, A. Surolia (eds.), Springer International Publishing Switzerland 2015.

Rahul Banerjee

1) Self – Complementarity in Protein Folding, Validation and Design



As protein polypeptide chains collapse during the process of protein folding, different parts of the polypeptide chain self recognize to form stable functional folds with densely packed hydrophobic interiors. The concept of complementarity which has been widely used to understand and predict biomolecular recognition has been applied to individual proteins. This has led to the identification of a finite number of ‘packing motifs’ which goes to constitute protein cores. Secondly, fairly stringent criteria in terms of electrostatic and surface complementarity, needs to be satisfied for buried residues (with respect to their neighbors) in order to support functionally viable folds. Inspired by the Ramachandran Plot, we have proposed a Complementarity Plot, which could find useful applications in protein validation and design. These computational tools have also been used to study the protein unfolding in the case of cyclophilin. This body of work has been reported in the following publications:

Basu, S., Bhattacharyya, D. & Banerjee, R. (2011) Mapping the Distribution of Packing Topologies within Protein Interiors Shows Predominant Preference for Specific Packing Motifs, *BMC Bioinformatics*, **12:195**

Basu, S., Bhattacharyya, D. & Banerjee, R. (2012),. Self – complementarity within proteins: bridging the gap between binding and folding. *Biophysical Journal*, **102**: 2605 – 2614

Basu, S., Bhattacharyya, D., & Banerjee, R. (2014) Applications of complementarity plot in error detection and structure validation of proteins. *Indian Journal of Biochemistry & Biophysics*. **51**, 188 – 200.

Roy, S., Basu, S., Datta, A.K., Bhattacharyya, D., Banerjee, R., & Dasgupta, D. (2014) Equilibrium unfolding of cyclophilin from *leishmania donovani*: characterization of intermediate states. *International. Journal. of Biological. Macromolecule*. 2014, **69**, 353-360

Roy S, Basu S, Dasgupta D, Bhattacharyya D, Banerjee R (2015) The Unfolding MD Simulations of Cyclophilin: Analyzed by Surface Contact Networks and Their Associated Metrics. *PLoS ONE* 10(11): e0142173.

Future Plans: a) To computationally design a protein which is a peptidyl prolyl cis trans isomerase using the tools described above and experimentally confirm that the design targets have been met. b) Three distinct folds cyclophilin, parvulin and FKBP converge to the same function. Use a combination of x-ray crystallography, spectroscopy and computation to understand the invariant features in their structure which can support the same function.

2) Drug targeting in *Leishmania spp*

Leishmaniasis, a broad spectrum of diseases caused by *leishmania spp.* is widely prevalent in the Indian subcontinent. With the emergence of resistant strains it becomes imperative to continue the search for novel therapeutics to combat the disease. In this project we have employed bioinformatics, x-ray crystallography and cell screening to identify drug targets in the parasite and known drugs which could serve as anti-leishmanials. This body of work has been reported in the references given below:

Waugh, B., Ghosh, A., Bhattacharyya, D. Ghoshal, N. & Banerjee, R. (2014) In silico work flow for scaffold hopping in Leishmania *BMC Research Notes*, **7**:802

Waugh B., Sen U. & Banerjee R. (2015) Crystal Structure of Phosphoglucomutase From *L. Major* at 3.5 Å Resolution, *Biochimie*, **121**: 102 – 111

Future Plans a) To screen prospective drugs identified in the bioinformatics as antileishmanials and also test for synergism between the drugs. Initial results appear to be very encouraging. b) Solve crystal structures of proteins from the Leloir and Isselbacher pathways unique to the parasite for drug targeting.

3) Philosophical Studies in Consciousness

The problem of consciousness has reemerged has a genuine scientific problem. Currently, there exists a wide divergence of views with regard to the ontology and status of consciousness in the natural order. The work primarily focuses on the Indian philosophical models of the conscious mind, both classical and modern with a view to understand theoretical scenarios which could make a contribution to the current discourse on consciousness. The relevant references are :

Banerjee, R. (2008) Buddha and the Bridging Relations, *Progress in Brain Research* Volume 168, Elsevier Amsterdam.

Abhidhamma Principles in the Theory and Practice of Meditation. Banerjee, R. ISBN : 9789380336596 , 2012, Mahabodhi Book Agency.

Indian Philosophy and Meditation: Perspectives on consciousness. Banerjee R and Chatterjee A, Routledge, Taylor and Francis Group Publication, 2017

Future Plans a) Developing theoretical models of the 'internal state' inspired by the Indian philosophical tradition. b) Develop textbooks for Indian psychology and manuals for the alleviation of depression using mindfulness techniques.

Udayaditya Sen



Professor 'G'

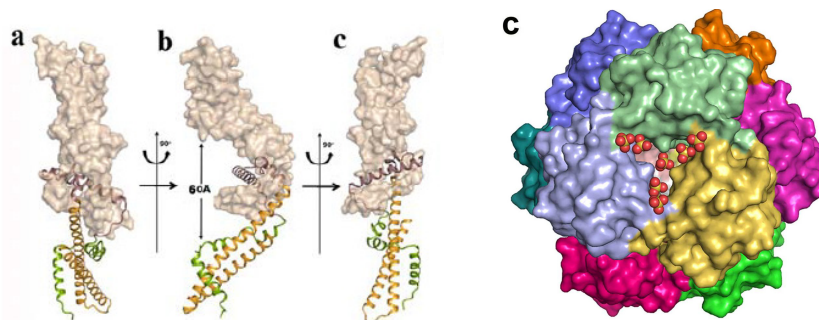
Ph. D: Saha Institute of Nuclear Physics, 1999

Postdoctoral research: The Scripps Research Institute, California, USA

Postdoctoral research: University of Southern California, California, USA

Research Activities

Last five years several structures have been solved from my lab. These include structures with novel folds, complicated protein assembly or protein:preprotein complexes, protein:substrate analogue complexes and atomic resolution structures. Among them the structure of Psu and the cage structure of an Acylphosphatase drew much attention. Psu, a capsid decoration protein of bacteriophage P4, acts as an antiterminator of Rho-dependent transcription termination in bacteria. Currently, two types of transcription termination inhibitor are known, namely Psu and YaeO and crystal structure of both of them have been solved from my lab. Structure of Psu, solved by Hg-SAD method at 2Å resolution, revealed a novel fold with a unique knotted dimerisation. The 12-meric nano-cage (~8 nm) structure of acylphosphatase from *Vibrio cholerae*O395 (Vc-AcP), coupled with studies in solutions illuminate the basis for the formation of the cage, while a single (Cys20→Arg) mutation (Vc-AcP-C20R) transforms Vc-AcP to a potent enzyme, but disrupts the assembly into a trimer.



My lab is also engaged in structural studies on proteins implicated in phosphorylations/dephosphorylations like acylphosphatases, LMW PTPs and Sugar Kinases. Atomic resolution (1.45Å) structure of Vc-PTPa with a substrate mimicry MOPS, elucidates the role of residues involved in substrate binding and detail interactions at the active site. Phosphorylation of Fructose and Ribose (by

Fructokinase and Ribokinase) is the first step in sugar metabolism. We have proposed a mechanism of fructose phosphorylation, for the first time, based on the crystal structure of apo and ligand bound fructokinase coupled with enzyme kinetics of WT and mutant fructokinase. Large scale conformational motion upon sugar binding along with surface charge redistribution provides a mechanism of high fidelity of the reaction.

Currently, I am working with small heat shock proteins Hsp31, Hsp15, Hsp16.5 and GrpE. Crystal structures and biochemical studies indicate novel mechanistic properties of Hsp31 and Hsp15. c-di-GMP is a global second messenger cellular level of which switches the controls between motile to biofilm state. Structure of a c-di-GMP phosphodiesterase has been solved in apo and c-di-GMP bound form. While VpsR, a novel transcriptional regulator that controls the development of biofilms in *V. cholerae* have been cloned. The central AAA+ domain has been cloned tested for ATPase activity and crystallized in apo and ANP-PNP bound form.

Selected Publications (last five years)

1. Das S, Roy Chowdhury S, Dey S, **Sen U** (2017) *PLoS ONE* 12(2): e0172629
2. Majumder S, Khamrui S, Banerjee R, Bhowmik P, **Sen U**. (2015) *BBA*. 2015 1854(1): 55-64.
3. Paul R, Patra MD, **Sen U**. (2015) *Adv Exp Med Biol.*; 842:293-307.
4. Nath S, Banerjee R, **Sen U**. (2014) *BBRC* 450(1): 390-5.
5. Nath S, Banerjee R, **Sen U**. (2014) *J Mol Biol.* 426(1):36-8.
6. Biswas M, Dey S, Khamrui S, **Sen U**, Dasgupta J. (2013) *PLoS One*. 8(9):e73923.
7. Ranjan A, Sharma S, Banerjee R, **Sen U**, Sen R. (2013) *Nucleic Acids Res.* 41(14):6839-56.
8. Banerjee R, Nath S, Ranjan A, Khamrui S, Pani B, Sen R, **Sen U**. (2012) *J Biol Chem.* 287(53):44667-75.
9. Das S, Ghosh S, Dasgupta D, **Sen U**, Mukhopadhyay D. (2012) *BBRC*. Jul 21
10. Majumder S, Khamrui S, Dasgupta J, Dattagupta JK, **Sen U**. (2012) *BBA*. 1824(7):882-90.

Thesis awarded for PhD (during 2012 – June 2017)

1.	Sudip Majumder	Faculty in Amity Univ, Gurgaon
2.	Samir Das	Postdoc Univ of British Columbia
3.	Ramanuj Banerjee	University of Michigan, USA
4.	Seema Nath	
5.	Rakhi Paul	Faculty, Bethune College

Summarized Carrier Profile

1. Name: Partha Saha
Present Position: Professor 'G'
Crystallography and Molecular Biology Division
Phone Extension: 1309
Mobile: 94330 35979



2. Education:

M.Sc. Biotechnology. Indian Institute of Technology, Bombay. 1989. India. 1st Class.
Ph.D. Jadavpur University, Kolkata, India. 1995

Membership of professional bodies: Society for Biological Chemists (India)
Indian Society of Cell Biology

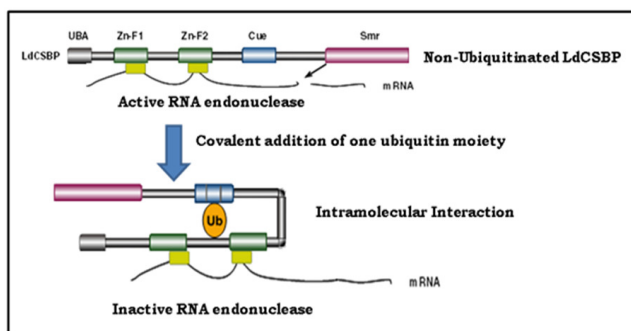
3. Research:

Major area of specialization: Biochemistry, Molecular Biology, Cell Biology.

Field of Interest: Regulation of DNA replication and cell cycle in eukaryotes.

Major Findings:

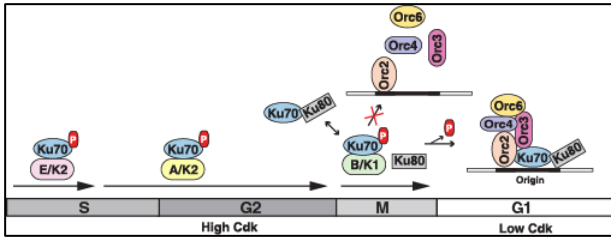
- In nearly complete absence of transcriptional regulation, mRNA turnover is primarily responsible for differential gene expression in disease causing trypanosomatid parasites. In these organisms, periodic accumulation of S-phase messages during cell cycle is determined by



the presence of one or more copies of a conserved CAUAGAAG octamer motif in their untranslated regions. We have shown that a multi-domain cycling sequence binding protein LdCSBP from *Leishmania donovani* binds specifically to the octamer containing RNAs via its uniquely arranged CCCH type Zn-fingers and degrades them through its Smr endonuclease domain. Interestingly, the

protein is modified by the incorporation of a mono-ubiquitin residue at its Zn-finger domain and the interaction of its CUE domain with the ubiquitinated Zn-finger domain is responsible for inhibition of its riboendonuclease activity. The findings establish an inhibitory mechanism of RNA cleavage in eukaryotes through ubiquitination mediated intra-molecular interaction among domains of an enzyme. Furthermore, the riboendonuclease activity is inhibited by anti-leishmanial drug paromo-mycin suggesting that the regulation of RNA metabolism could be a target of the drug.

- Accurate replication of DNA in eukaryotic cells is controlled by a cell cycle dependent licensing mechanism that allows formation of a competent pre-replication complex only after mitotic segregation of sister chromatids into daughter cells. Intriguingly, Ku – a DNA repair protein is also involved in the process but its regulation remained long unknown.



Recently, we have shown that the periodic modulation of replication related function of Ku is dependent on reversible phosphorylation of its Ku70 subunit by cell cycle kinases. The findings establish further insight regarding the regulatory mechanism of replication initiation involving multi-functional Ku protein, which is critical for genomic stability.

Students Guiding: Ph.D. students : **Completed 2** **Thesis submitted 1**
 Postdoctoral Fellow : **2**

4. Future Plan:

- **Regulation of gene expression at post-transcriptional level in eukaryotes:** the proposed work will involve the elucidation of role of *cis*-elements in the UTR of mRNAs of several mammalian cell cycle related genes at molecular and cellular level using various techniques of cell and molecular biology and high-throughput approaches such as next generation sequencing and proteome analysis.
- **Regulation of cell cycle related function of Ku protein:** The study of DNA repair protein Ku in replication licensing will be carried out in genomic scale via high throughput approaches like ChIP-seq to elucidate any differential relationship of its involvement with the origin-uses in a spatio-temporal manner. Our preliminary results also implicate that there could be novel functional interaction of Ku protein with the cell cycle modifier polo-like kinase 1 (Plk1), which we propose to elucidate in detail.

5. List of Important Publications during 2012-2016 (Total 16):

- [1] Mukherjee, S., P. Chakraborty and P. Saha (2016) Phosphorylation of Ku70 subunit by cell cycle kinases modulates the replication related function of Ku heterodimer. *Nucleic Acids Res* **44**:7755-65.
- [2] Ganguly, B. N., V. Verma, D. Chatterjee, B. Satpati, S. Debnath and P. Saha (2016) Study of Gallium Oxide Nanoparticles Conjugated with beta-Cyclodextrin: An Application To Combat Cancer. *ACS Appl Mater Interfaces* **8**:17127-37.
- [3] Guha, K., S. Das and P. Saha (2014) Lys-413 of S-phase mRNA cycling sequence binding protein from *Leishmania donovani* (LdCSBP) is modified through monoubiquitination that is responsible for inhibition of its ribonuclease activity. *J. Biochem. Biophys.* **51**:559-566.
- [4] Guha, K., D. Bhandari, T. Sen and P. Saha (2014) Ubiquitination-mediated interaction among domains is responsible for inhibition of RNA endonuclease activity of mRNA cycling sequence binding protein from *L. donovani* (LdCSBP). *Parasitol Res* **113**:2941-9.
- [5] Banerjee, S., S. Chaudhuri, A. K. Maity, P. Saha and S. K. Pal (2014) Role of Caffeine in DNA Recognition of a Potential Food-Carcinogen Benzo[a]pyrene and UVA induced DNA damage. *J. Molecular Recognition* **28**:510-520.
- [6] Maity, A. K. and P. Saha (2012) The histone acetyl transferase LdHAT1 from *Leishmania donovani* is regulated by S-phase cell cycle kinase. *FEMS Microbiol Lett* **336**:57-63.

Name: Sampa Biswas



Academic Profile:

M.Sc in Biophysics and Molecular Biology, CU
Ph.D from Bose Institute, Kolkata, 1995
1995-1996: Post-doc, Central Drug Research Institute, Lucknow.
1996-1997: Post-doc, Saha Institute of Nuclear Physics.
1997- till date : Faculty Saha Institute of Nuclear Physics.

Awards, honours and distinctions:

Fellow, West Bengal Academy of Science and Technology (WAST).

Life member of Indian Physical Society and Indian Crystallographic Association

Teaching:

1. Post-M.Sc (Biophysical Science) teaching program of SINP.
2. M.Sc Biophysics and Molecular Biology Department, Calcutta University (2009-2015).

Essential strength of research/development output:

Area of research interest: Structural Biology, Structure-based protein engineering, Protein crystallography and molecular modeling.

Current research projects (2012-2016):

During this period, my main focus is on understanding the regulation mechanism of C1A cysteine proteases through structural, mutational, biochemical and biophysical studies. Our group has persuaded the following three projects:

1. SCCA1 (squamous cell carcinoma antigen1) and MENT (myeloid and erythroid nuclear termination stage specific protein) mediated regulation of proteolytic activity of lysosomal cysteine proteases- biochemical, biophysical and structural studies
2. Structural insights into the effects of causative mutations of human cathepsin K responsible for bone deformations.
3. Role of pro-peptide part in folding and maturation of papain-like cysteine proteases

Future research/development plan:

Structure-based protein engineering to alter functional properties of proteases has already been explored with success in our laboratory. We would like to extend these endeavors by converging the expertise of structural and functional studies and recombinant DNA technology to attain a goal having more focus on applications of the engineered proteins.

The following proposed projects are higher level programs of our ongoing research activity which we intend to start in near future. We have already performed some back-ground work to evaluate the feasibility of the projects.

1. Imparting hemoglobinase (capability to degrade haemoglobin) activity in cysteine proteases by structure guided rational design.
2. Design and generation of potential inhibitor of falcipain 2, a malarial parasitic protease, from cross-class serpin inhibitors.

Publications (during 2012-2016)

1. "Mutation in the pro-peptide region of a cysteine protease leads to altered activity and specificity - A structural and biochemical approach" Sruti Dutta, Debi Choudhury, Sumana Roy, Jiban Kanti Dattagupta and **Sampa Biswas**. *PLoS ONE* (2016) 11(6): e0158024.
2. "N-acyl - Schiff base complex as enzyme inhibitor of hen egg white lysozyme: a crystallographic and spectroscopic study" Banabithi Koley Seth, Aurkie Ray, **Sampa Biswas** and Samita Basu. *Metallomics* (2014), **6**, 1737-1747.
3. "Enhancement of proteolytic activity of a thermostable papain-like protease by structure-based rational design" Sruti Dutta, Jiban Kanti Dattagupta and **Sampa Biswas**. *PlosOne* (2013) May 3;8(5):e62619.
4. "Protein interactions of Merocyanine 540: spectroscopic and crystallographic studies with lysozyme as a model protein" Piyali Mitra, Mousumi Banerjee, **Sampa Biswas**, Samita Basu. *Journal of Photochemistry and Photobiology B: Biology* (2013) **121** 46–56.
5. "The structure of a thermostable mutant of pro-papain reveals its activation mechanism" Sumana Roy, Debi Choudhury, Pulakesh Aich, Jiban K Dattagupta and **Sampa Biswas**. *Acta Crystallographica- Biological Crystallography* (2012) **D68**, 1591–1603.
6. "Expression of recombinant human cathepsin K is enhanced by codon optimization" Sumana Roy, J.K. Dattagupta, **Sampa Biswas**. *Process Biochemistry* (2012) **47**, 1944–1947.

H. Raghuraman

Associate Professor-E,
Crystallography & Molecular Biology Division
h.raghuraman@saha.ac.in



Education:

Ph.D.: In Life Sciences and Biophysics, Centre for Cellular and Molecular Biology (CCMB), India (2004), Supervisor: Dr. Amitabha Chattopadhyay

M.Sc. (Medical Biochemistry): University of Madras, India (1997)

B.Sc. (Biochemistry): University of Madras, India (1995)

Positions Held:

Associate Professor-E: Saha Institute of Nuclear Physics, India (December 2014 – present)

Research Scientist: The University of Chicago, USA (May 2010 – December 2014)

Post-doctoral scholar: The University of Chicago, USA (July 2006 – April 2010)

Research Associate: CCMB, India (April 2005-May 2006)

Awards and Honors:

- “Member of the Jury Committee 2017” for Vidyarthi Vigyan Manthan (VVM)-a national level talent program jointly organized by Vigyan Prasar, Department of Science and Technology, Govt. of India, National Council of Educational Research & Training (NCERT), Govt. of India
- “SERB-Early Career Fellowship” Department of Science and Technology, Govt. of India (2016-17)
- Delivered ~20 invited seminars nationally and internationally
- “IUPAB Travel Fellowship” to participate in the 15th IUPAB & 5th EBSA International Biophysics Congress 2005 held at Montpellier, France
- “Young Scientist Award” of the Indian Biophysical Society (2005)
- Research Associate Fellowship, Council of Scientific and Industrial Research, Govt. of India (April 2005-June 2006)
- Senior Research Fellowship, Council of Scientific and Industrial Research, India (2003-March 2005)
- Senior Research Fellowship, University Grants Commission, Govt. of India (2001-2003)
- Junior Research Fellowship, University Grants Commission, Govt. of India (1999-2001)
- University Rank 2nd in M.Sc. Medical Biochemistry, University of Madras
- University Rank 8th in B.Sc. Biochemistry, University of Madras

Area of Research & Future Interests:

The focus of my thesis work involved understanding the intricate network of lipid-protein interactions in membranes utilizing the hemolytic peptide melittin as a model system and sensitive fluorescence approaches. I have addressed some of the basic and fundamental issues concerning the role of hydration, electrostatics, aggregation, orientation and the presence of specific lipids like polyunsaturated lipids and cholesterol in melittin-membrane interactions. My post-doctoral research is mainly focused on understanding the structural dynamics involved in C-type inactivation gating mechanisms in potassium channels and the structural transition associated with the voltage sensor movement in voltage-sensitive proteins. My current research is focused on understanding the activation gating mechanisms of potassium and magnesium ion channels, molecular basis of ion permeation and selectivity and lipid-dependent gating mechanisms. We will utilize site-directed fluorescence approaches, site-directed spin labeling & electron paramagnetic resonance (SDSL-EPR), liposome patch clamp and X-ray crystallography to understand the structural dynamics of membrane proteins in general, and ion channels and transporters, in particular.

Publications since 2012:

1. Kratochvil, H.T., Carr, J.K., Matulef, K., Annen, A.W., Li, H., Maj, M., Ostmeyer, J., Serrano, A.L., **Raghuraman, H.**, Moran, S.D., Skinner, J.L., Perozo, E., Roux, B., Valiyaveetil, F.I., and Zanni, M.T. (2016) Instantaneous ion configurations in the K⁺ ion channel selectivity filter revealed by 2D IR spectroscopy. *Science* 353: 1040-1044.
2. Pillai, V.B., Samant, S., Sundaresan, N.R., **Raghuraman, H.**, Kim, G., Bonner, M.Y., Arbiser, J.L., Walker, D.I., Jones, D.P., Gius, D., and Gupta, M.P. (2015) Honokiol blocks and reverses cardiac hypertrophy in mice by activating mitochondrial Sirt3. *Nat. Commun.* 6: 6656.
3. **Raghuraman, H.**, Islam, S., Mukherjee, S., Roux, B., and Perozo, E. (2014) Dynamics transitions at the outer vestibule of the KcsA potassium channel during gating. *Proc. Natl. Acad. Sci. USA* 111: 1831-1836.
4. White, E., **Raghuraman, H***, Perozo, E., and Glotzer, M. (2013) The mechanism of microtubule bundling by central spindle during cytokinesis. *J. Biol. Chem.* 288: 19785-19795.
5. **Raghuraman, H.**, Cordero-Morales, J., Jogini, V., Kollwe, A., and Perozo, E. (2012) Mechanism of Cd²⁺ coordination during slow inactivation in potassium channels. *Structure* 20: 1332-1342.
* equal contribution

Society Memberships:

- Society of Biological Chemists, India
- Indian Biophysical Society – Life member
- Indian Photobiology Society – Life member
- Indian Academy of Neurosciences – Life member

National Level Academic Review

Chemical Sciences Division (CSD)

*A report for the period of 2012 - **June 2017***

Present Staff

Scientific/Faculties (8)	Technical / Sc. Assistants (3)
Amitabha De Senior Prof. H	Ajay Das SA-F
Samita Basu, Senior Prof. H+ & Head	Chitra Raha SA-E
Susanta Lahiri, Senior Prof. H+	Avijit Shome SA-D
Munna Sarkar, Prof. G	
Maitreyee Nandi, Prof. G	Administrative / Auxilary (3)
Padmaja Prasad Mishra, Associate Prof. E	Subir Bandyopadhyay Superintendent
Montu K. Hazra Associate Prof. E	Bablu Ram Tech E
Dulal Senapati, Associate Prof. E	Dipak Ram Tech B
	Jitendra Nath Ray Tech B
Faculty Superannuated (1)	
Soumen Basak, Senior Prof. H (2012)	

Present Postdoctoral Fellows (PDFs)

	Name of PDFs	Year of Joining
1	Munmun Bardhan	2015
2	Arnab Maiti	2016
3	Uttam Pal	2016

Present Research Fellows (RFs)

	Name of RFs	Year of joining (PMSc)	Ph.D Supervisor
1.	Chaitrali Sengupta	2011 (thesis submitted)	Samita Basu
1	Swati Goswami	2011 (thesis submitted)	Munna Sarkar
2	Sourav Ghosal	2012	Montu K. Hazra
3	Maireyee Bhattacharya	2013	Dulal Senapati
4	Avishek Sau	2013	Samita Basu
5	Tapas Pal	2012	Padmaja P. Mishra
6	Sudeshna Das Chakrabarty	2013	Dulal Senapati
7	Sandip Kr Dey	2015	Dulal Senapati
8	Dibyasree Choudhury	2015	Susanta Lahiri
9	Samrat Basak	2015	Padmaja P. Mishra

PhD degree awarded (2012—present: 20)

Sl No.	Name of RFs	Year	Ph.D supervisor	Present Occupation
1.	Brotati Chakraborty	February 2012, Jadavpur University (JU)	Samita Basu	Assistant Professor in Chemistry, Bejoy Narayan Mahavidyalaya, Itachuna, Hooghly, WestBengal.
2.	Sutapa Mondal	November 2012, JU	Munna Sarkar	Research Associate, Department of Applied Chemistry, S. V. National Institute of Technology, Ichchhanath, Surat – 395007, Gujarat
3.	Manas Kumar Sarangi	February 2013, Calcutta university (CU)	Samita Basu	Assistant Professor, Department of Physics, IIT Patna, Bihar
4.	Mousumi Banerjee	March 2014, JU	Samita Basu & Abhijit Chakrabarti (CSD and B&SG)	DS Kothari Fellow, CU
5.	Binita Dutta	July 2014, CU	Susanta Lahiri	Post Doctoral Fellow at Central Power Research Institute (CPRI),
6.	Debabrata Nandi	November 2014, CU	Amitabha De (SINP) & Uday Ch. Ghosh and Arup Ghosh (Presidency College, Kolkata)	Post Doctoral Fellow at Dresden, Germany.
7.	Sreeja Chakraborty	December 2014, JU	Munna Sarkar	
8.	Kaustab Ghosh	May 2015, CU	Susanta Lahiri	PDF at Technical University of Delft, Netherlands

9.	Ankan Dutta Chowdhury	June 2015, CU	Amitabha De	PDF, National Chiao Tung University, Taiwan
10.	Sujay Ghosh	September 2015, CU	Samita Basu	PDF at Central Glass and Ceramic Research Institute, Kolkata
11.	B. H. VENKATARAM PAI	2016, Manipal	Maitreyee Nandy (CSD) & Prof. A. Krishnamoorthy, 11MIT, Manipal	Faculty, Civil Engineering Department, Manipal Institute of Technology, Manipal University
12.	Moupriya Nag	February 2016, CU	Soumen Basak	PDF at Bose Institute, Kolkata
13.	Piyali Mitra	February 2016, JU	Samita Basu	DST_SERB PDF at Indian association for the Cultivation of Science, Kolkata
14.	Kallol Bera	April 2016, CU	Soumen Basak	PDF at TIFR, Mumbai
15.	Ajoy Mandal	February 2016 (CU)	Susanta Lahiri	Technical assistant, Group-II, Controller of Examinations, University of Burdwan, WB
16.	Banabithi Koley Seth	September 2016, JU	Samita Basu	PDF at Technical University of Darmstadt, Germany
17.	Anupa Majumdar	June 2016, JU	Munna sarkar	PDF at IISER, Mohali
18.	Neha Rai	November 2016, CU	Sanghamitra raha (C&MB) and Munna Sarkar (CSD)	Postdoctoral Researcher, The Life Science Centre School of Science and Technology, Örebro University, Örebro, Sweden

19..	Nidhi Agnihotri	March 2017, CU	Amitabha De	Asiistant Professor in Chemistry, Kanoria P.G. College, Jaipur
20..	Amrit Krishna Mitra, Kolkata	April 2017, CU	Chandan Saha, School of Tropical Medicine and Samita Basu (CSD)	Assistant Professor & Head, Chemistry Department, Singur Government College, West Bengal

Ph.D thesis submitted (3)

	Name of RFs	Year	Ph.d Supervisor	Status
1.	Chaitrali Sengupta	November 2016	Samita Basu	Thesis reports received, waiting for viva-voce examination
2.	Swathi Goswami	March 2017	Munna Sarkar	
3.	Subhas Chandra Bera	April 2017	Padmaja P. Mishra	Postdoc at TIFR, Hyderabad

Ph.D thesis to be submitted (2)

	Name of RFs	Ph.D supervisor	Status
1.	Tapas Paul	Padmaja P. Mishra	Thesis will be submitted by July 31, 2017
2.	Sourav Ghoshal	Montu K. Hazra	Thesis will be submitted by July 31, 2017

Major Instruments in Chemical Sciences Division

Spectroscopy

UV-Vis spectrophotometer & one near IR absorption spectrophotometer

Fluorescence Spectrophotometer

Fourier Transform Infrared (FTIR) Spectrometer

CD spectropolarimeter

Picosecond Fluorescence Lifetime Measurement System (using TCSPC technique)

Nanosecond Flash Photolysis Setup for time-resolved absorption spectroscopy

Millisecond Stopped-Flow System for Absorption / Fluorescence study of reaction kinetics

Fluorescence Correlation Spectroscopy (In-house setup)

Femtosecond Fluorescence Up-Conversion kinetic spectrometer

Single-Molecule FRET

Optical Tweezer

Surface Enhanced Raman Spectroscopy (SERS) based Detection system

Dynamic Light Scattering,

Atomic Force Microscope

Electrochemistry

Cyclic Voltameter

Potentiostat/Galvanostat system for Electrochemical Analysis

Low-temperature (down to 10K) Resistivity Measurement setup

Chemical Analysis

Elemental Analyzer (CHNS) , Millipore water purifier, -85°C Deep Freezer, etc.

Nuclear & Radiochemistry

Inductively Coupled Plasma Optical Emission (ICPOES) Spectrometer

Inductively Coupled Plasma Mass Spectrometer (ICPMS) with GC, HPLC and Laser Ablation Attachments

HPGE Compton suppressed

HPGE-FALCON

HPGE –LEG

NAI (TL)

HPGE - We'll type

HPGE-Portable

Class 10000 Clean Room

Co60 radioactive source (Gamma irradiation chamber)

Radiation survey meters

Microwave digester

Gas phase dynamics

Molecular Beam Chamber

Research Highlights, Important Results and Future Plan of Chemical Sciences Division.

Research in the Chemical Sciences Division is wide-ranging and interdisciplinary, and addresses fundamental aspects of science. Overarching goals of the research projects include understanding of the excited state dynamics of complex phenomena using ultra fast spectroscopy and single molecule imaging, finding new functions for old drugs: Non Steroidal Anti-inflammatory Drugs (NSAIDs), different areas in Nuclear Chemistry, Radiochemistry and Green Chemistry, developing nanotechnology and novel advanced materials for a myriad of applications, unraveling problems associated with devising new, alternative sources of energy, neutron spectrometry and interaction, nano particle dosimetry and radiation safety.

Time-resolved spectroscopy within femtosecond to nanosecond time regime is being used extensively to study excited state dynamics on photoinduced electron transfer, proton transfer, etc with small organic molecules as well as to decipher the mode of intercalation of some common acridine derivatives with calf Thymus DNA. Similarly the results from laser flash photolysis experiments corroborated with magnetic field highlight the inter-radical separation distance between acridine derivatives and serum albumin proteins undergoing photoinduced electron transfer during binding. Moreover, steady-state and time-resolved spectroscopic studies supported by theoretical docking analyses on structure dependent hydrophobic and hydrophilic interactions of Schiff base complexes, comprising of different metal ions and ligands, with serum albumins as well as hen egg white lysozyme proteins emphasize the potentiality of less explored nickel complexes in drug-protein interactions. In recent years emphasis has been given on extension of the work using crystallography and STD NMR spectroscopy, synthesizing copper(II) and Nickel(II) Schiff base complexes which can act as efficient small perturbing agents for biomacromolecules by distinguishing the relation of the structures and functions of these complexes towards different model biomacromolecules and cell lines like HeLa and WI-38 and assessment of antibacterial efficacy of therapeutically important small molecules conjugated with gold nanoparticles. Very recently we have succeeded in synthesizing 'photoluminescent' carbon dots. As per our concern, this is a pioneering work, where the plausible molecular structure and the intrinsic mechanisms governing photoluminescence of carbon dots are explained by trapping seven visibly distinct coloured intermediates evolved during pyrolytic metamorphosis of citric acid (CA) with dopant Ru(III) as an indicator. The metamorphosis of Ru: carbon dots is monitored by characterizing each trapped intermediate using HR-TEM, DLS, XPS, XRD, $^1\text{H-NMR}$, FT-IR, and steady-state and time-resolved UV-visible and fluorescence spectroscopy as well as magnetic field effect. The photoinduced electron transfer ability of such carbon dots helps to develop their utility as quinone-sensor in live cells.

Copper complexes of Oxycam NSAIDs have been synthesized to study their biological applications. They form a new class of membrane anchors that require neither molecular recognition nor strength of interaction between interacting molecular partners, but still can effectively increase membrane fusogenic efficacy over the bare drugs. This new

class of membrane anchors is therefore a step ahead of traditional anchors that are based on two interacting molecular partners. DNA-binding with high base sequence specificity and apoptosis inducing properties have also been found for these complexes. Also, the copper complexes of traditional NSAIDs have been found to cause structural alterations upon interaction with chromatin/histone that makes them exert their effect at the epigenomic and genomic level.

Au-Polyaniline based conducting nano-composite has been utilized for bio-sensing of glucose, DNA and protein, using different electrochemical techniques and also for detecting the positional effect of single base mismatch in oligonucleotides. PEDOT-MnO₂ and graphene based materials have been used to fabricate supercapacitors of high specific capacitance. A non-enzymatic electrochemical biosensor has been fabricated for cholesterol detection, having a distinct advantage over other conventional enzymatic processes. Chemically converted Graphene modified with β -CD, being hydrophilic, electroactive and high surface area material, provides a platform for the electrochemical detection of cholesterol using Methylene Blue as redox indicator. Graphite nanoplatelet (GNP)/conducting polymer (poly(3,4-ethylenedioxythiophene)-poly(styrenesulfonate)) (PEDOT:PSS) composites were synthesized for their application as highly efficient electromagnetic interference (EMI) shielding material (SE) in the X-band frequency region.

A single molecule and ensemble spectroscopic study of dynamics of double stranded DNA and other DNA structural motifs were carried out. Effect of interaction of DNA with different nano particles as well as graphene oxide was carried out using the above methods. The following results were obtained. i). *Conformational changes and complete unzipping of dsDNA by surface modified Gold Nanoparticles (The Journal of Physical chemistry B, 2016)*. In this work the interaction of dsDNA with surface modified gold nano particles was studied. A collaborative effect of the nanoparticles resulted in structural changes e.g. compaction and strand separation depending on the size and hence the charge on the AuNPs. ii). *Bubble dynamics and DNA flexibility in presence of base pair mismatch (Manuscript Published In RSC Advances and in Nanoscale)*. Dynamics of the thermally induced DNA bubble formation shows spontaneously zipping- unzipping rate which follows multistate relaxation kinetics. The nature of bubble has been investigated using small DNA containing 23 nucleotides and having preferred nucleotide sequence nearly identical to that of the transcription initiation sequence. The selective introduction of base pair mismatch for creation of melting bubble affects the local base stacking, along with the base pairing. iii). *Chaotic Dynamics During the Restricted Branch Migration of IHF Bound Holliday Junctions due to Applied Force: A smFRET study*. The enhanced rigidity and reduced flexibility, that a Holiday junction experiences upon binding to a DNA binding/Bending Protein, IHF have been monitored. Using single molecule FRET technique, detection of the isomerization dynamics in presence of applied force becomes possible. iv). *Single molecule FRET Studies of Hybridization mechanism during the noncovalent adsorption and desorption of DNA on Graphene Oxide. (Manuscript Published in the Journal of Physical chemistry B)*. This provides the insight about the interaction of DNA with low dimensional material like 'Graphene

Oxide' (GO) to give a detail hybridization mechanism during the adsorption and desorption of DNA on its surface.

Recently, different architectures of nanomaterials which include tunable gold nano-flowers, silver nano-wires, selenium nano-spheres, intercalated nano-prism, branched gold nano-crystals, and porous silver nano-materials have been developed. The main /results areas probed:

a) Standardization of nanotemplated growth technique for overgrowth anisotropic SERS active nanomaterials synthesis. b) Controlled nanowire synthesis with aspect ratio ~1000 can replace carbon nanotube for their flexibility and giant conductivity. c) Miniaturized electroanalytical instrument for cost effective blood profiling. d) Synthesized bimetallic noble metal nanoparticle shows effective and selective killing of tuberculosis bacteria. e) New generation mesoporous silica nanoparticle (MSN) for pH induced non-toxic drug delivery. f) Newly synthesized hedgehog gold nanoparticle with high molecular weight non toxic polymer screening for long retention in blood vessel with ~5000K nanoscale thermalization. g) Establishment of new field "Magnetic Field Enhanced Spin Dynamics".

The nuclear and radiochemistry group is engaged in various activities. For the first time non-destructive method have been designed to determine K content of ancient glass beads which eventually tells about the origin of glass bead. Contribution have made in Radio-Green Chemistry experiments. Ionic liquids and other green reagents have been used to separate no-carrier-added clinically important radionuclides like ^{61}Cu , ^{62}Zn , ^{97}Ru , $^{95,96}\text{Tc}$, ^{111}In and ^{109}Cd . An effective separation of ^{163}Ho was designed from ^{163}Er which has implications in neutrino mass measurement. Another important program of nuclear and radiochemistry group is measurement of naturally occurring radioactive material in Sundarban and Punjab state in collaboration with University of Calcutta and Panjab University.

The decomposition of isolated carbonic acid (H_2CO_3) molecule into CO_2 and H_2O ($\text{H}_2\text{CO}_3 \rightarrow \text{CO}_2 + \text{H}_2\text{O}$) is prevented by a large activation barrier (>35 kcal/mol). Nevertheless, it is surprising that the detection of the H_2CO_3 molecule has not been possible yet in the Earth's atmosphere and hunt for the free H_2CO_3 molecule has become challenging not only in the Earth's atmosphere but also on Mars. In view of this fact, we first study the instability of H_2CO_3 molecule in presence of water (H_2O), formic acid (FA), acetic acid (AA) sulfuric acid (SA) and hydroperoxide radical (HOO), detected in the Earth's atmosphere. It is seen from this study the vapor phase of H_2CO_3 molecule is unstable in presence of H_2O , FA and AA. Moreover, we also study the energetics and kinetics of the OH radical-initiated H_2CO_3 degradation reaction ($\text{H}_2\text{CO}_3 + \text{OH} \rightarrow \text{HCO}_3 + \text{H}_2\text{O}$) to interpret the loss of the H_2CO_3 molecule in the Earth's atmosphere, as the OH radical is known as the atmospheric detergent. Importantly, it is seen from these two studies that, although the atmospheric concentration of the OH radical is substantially lower than the concentrations of the H_2O , FA, AA in the Earth's atmosphere, but nevertheless, the OH radical-initiated H_2CO_3 degradation reaction has significant impact, especially, towards the loss of H_2CO_3 molecule in the Earth's atmosphere. In contrary, although the catalytic efficiencies of SA, FA and AA upon the H_2CO_3 decomposition

reaction are similar to each other and the concentrations of both the SA and OH radical in the Earth's atmosphere are more-or-less equal to each other, but nevertheless, the SA-assisted H_2CO_3 decomposition reaction cannot compete with the OH radical-initiated H_2CO_3 degradation reaction.

Effect of nuclear mean field and multiple preequilibrium mechanisms in neutron emission from heavy ion reaction has been studied in the energy range of 10 MeV/amu to 30 MeV/amu. For the available sets of double differential neutron data, e.g., ^{20}Ne and ^{12}C induced reaction on ^{165}Ho system, the model has been observed to reproduce the measured data well. Whole body dose distribution and organ absorbed dose determined using measured neutron distribution from $^{12}\text{C} + \text{C}$ reaction at 12 MeV/amu. Our study showed that ~21% of the total dose is contributed by neutrons above 20 MeV and average quality factor of the neutrons from this reaction is ~10.2. Synthesis and influence of silver nano-particles in dose enhancement for gamma irradiation is being studied.

Future Plan

Potential Application of Softmatter & Small Molecules: Fabrication, Interaction and Conformational Dynamics: The future research activity of chemical sciences involves fabrication, interaction and conformational dynamics of soft-matter and small molecules with the aim to provide a practical framework for the wider understanding of their potential applications for a targeted research from which our society will be benefited. Based on initial studies, targets would be set for applications of the fabricated materials in real systems that include radioisotope doped nanoparticle driven drug delivery, DNA damage repairing, pollution control in upper atmosphere and development of low-coast, user-friendly innovative sensors for precise understanding of the physico-chemical basis behind their extreme environmental adaptations.

Molecular Insights of designing drug-delivery systems for cancer: Different types of nanomaterials and small drug molecules would be designed to fabricate composite materials to target not only a specific type of cancer cell but also to manipulate different physico-chemical conditions to deliver drug molecules according to our desire. We also propose to study the effect of several drug delivery vehicles e.g. using different host guest systems, liposomes etc.

Based on the preliminary outcomes on cancer cell specific drug delivery systems, we shall proceed towards *in vivo* studies. Composite materials with programmable drug delivery efficiency that remains stable in physiological condition for long retention time and therapeutic DNA will be delivered to study their effect in animal body. This unique study will allow us to elucidating the molecular basis of different cancers and designing of better diagnostic tools for early detection and improved drug and drug delivery system for targeted delivery with minimal damage to the normal cells.

Studies across the energy scale, from sub eV to GeV: The future research activity of Nuclear and Radiochemistry Laboratory of Chemical Sciences Division is to explore fundamental aspects of production of isotopes in different energy scale, from sub eV to

GeV, development of their separation method and understanding the fundamental principle of working with few atoms. A new and unique Compton suppressed system based on clover detectors will be installed to play with sub-pico curie level of radioactivity. New ICPMS system will be installed (with LASER based ionization chamber) which will detect parts per trillion level of impurities. Cross section and yield data of clinically important radioisotopes produced through different nuclear reactions will be determined. Yield of radionuclides (especially pure α/β emitting radionuclides) in a complex and thick target matrix will be determined. Attempt will be made to discover new radionuclides (and even new elements) in transactinide region. The target will be the augmentation of trace analysis laboratory with quadrupole mass spectrometry, TXRF and other state-of the art instruments, development of radiochemical methodologies, development of capacity for sub-pico curie determination of radionuclides and creation of physical and chemical data bank for production and separation of radionuclides produced by the impact of projectiles of different energy regime.

List of Publications (2012—present):

(Total number: 165 [Peer Reviewed Journals: 161 + Book Chapter: 4]) Total Impact Factor (I.F.) = 398.884; citation = 946

2017

1. Nidhi Agnihotri, Pintu Sen, Amitabha De* and Manabendra Mukherjee, “Hierarchically designed PEDOT encapsulated Graphene-MnO₂ nanocomposite as Supercapacitors”, *Materials Research Bulletin*, 88, 218-225, 2017 (I.F. 2.435, citation =1).
2. Sujay Ghosh, Amrit Krishna Mitra, Uttam Pal, Samita Basu*, Chandan Saha, “Evidence of two structurally related solvatochromic probes complexed with β-cyclodextrin by using spectroscopic methods”, *Journal of Molecular Structure*, 1130, 810-817, 2017 (I.F. = 1.602)
3. Chaitrali Sengupta, Manas Kumar Sarangi, Abhishek Sau and Samita Basu*, “Micellar control over tautomerization and photo-induced electron transfer of Lumichrome in the presence of aliphatic and aromatic amines: a transient absorption study”, *Methods & Applications in Fluorescence*, 5, 014008, 2017. (I.F. = 2.429)
4. Chaitrali Sengupta, Piyali Mitra, Banabithi Koley Seth, Debabrata Mandal[#] and Samita Basu*, “Electronic and spatial control over the formation of transient ion pairs during photoinduced electron transfer between proflavine–amine systems in a subpicosecond time regime”, *RSC Advances*, 7, 15149 – 15157, 2017. (I.F. = 3.289)
5. Kakoli Banerjee, Nabanita Naskar, Dibyasree Choudhury, Susanta Lahiri, Trace analysis at the backdrop of women welfare: assessment of heavy metals in Vermillion (Accepted). (I.F. = 0.145)
6. Moumita Maiti, Susanta Lahiri, Deepak Kumar, Dibyasree Choudhury, Separation of no-carrier-added astatine radionuclides from □-particle irradiated lead bismuth eutectic target: A classical method, *Applied Radiation and Isotopes* 127, 227-230, 2017 (I.F. = 1.128)
7. Deepak Kumar, M Maiti, Susanta Lahiri, Production of Pd radionuclides from natural niobium and its purification simulating the ^{nat}Nb(¹¹B, xn)^{100,101}Pd reaction, *J. Radioanal. Nucl. Chem.* (DOI 10.1007/s10967-017-5286-y, (I.F. = 1.282, citation = 1)
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**PAPERS PRESENTED/APPEARED AT
CONFERENCES/SYMPOSIA
(01.01.2012 TO 31.12.2016)**

1. Dibyasree Choudhury, Susanta Lahiri, Estimation of α -emitting polonium radionuclides in proton irradiated lead bismuth targets by LSC-TDCR method, The Latest Advances in Liquid Scintillation Spectrometry (LSC-2017), May 1-5, 2017, Copenhagen, Denmark
2. Susanta Lahiri, Production of astatine from LBE, LIEBE coordination meeting, March 22, 2017, IPUL, Latvia (**Invited talk**, delivered through telephone)
3. Susanta Lahiri, Radium to radium: 100 years cycle, Eruption of Radionuclides in Imaging and Therapy, organized by Nuclear Medicine Physicist Association of India February 25-26, 2017, Kolkata (**Invited talk**)
4. Deepak Kumar, Moumita Maiti, Susanta Lahiri, Production of Pd radionuclides from natural niobium and its separation simulating the $^{nat}\text{Nb}(^{11}\text{B},\text{xn})^{100,101}\text{Pd}$ reaction, 13th DAE-BRNS Nuclear and Radiochemistry Symposium (NUCAR-2017), KIIT University, Bhubaneswar, Odisha, India, February 6-10, 2017 .
5. Kalpita Ghosh, Nabanita Naskar, Dibyasree Choudhury, Susanta Lahiri, Separation of no-carrier-added ^{88}Zr from proton induced bulk yttrium target by naturally synthesized hesperidin, 13th DAE-BRNS Nuclear and Radiochemistry Symposium (NUCAR-2017), KIIT University, Bhubaneswar, Odisha, India, February 6-10, 2017.
6. Nabanita Naskar, Susanta Lahiri, Punarbasu Chaudhuri, Alok Srivastava, The optimization of counting time in NORM measurement, 13th DAE-BRNS Nuclear and Radiochemistry Symposium (NUCAR-2017), KIIT University, Bhubaneswar, Odisha, India, February 6-10, 2017.
7. Moumita Maiti, Susanta Lahiri, Deepak Kumar, Pritam Chakraborty, Study of low energy proton induced reaction on lead-bismuth eutectic target, 61st DAE-BRNS Symposium on Nuclear Physics, Saha Institute of Nuclear Physics, December 05-09, 2016.
8. M Maiti, S Lahiri, D Kumar, D Choudhury, A Singh, Low energy α -particle induced reaction on thick lead-bismuth eutectic target, 61st DAE-BRNS Symposium on Nuclear Physics, Saha Institute of Nuclear Physics, Kolkata, December 05-09, 2016.
9. Deepak Kumar, Moumita Maiti, and Susanta Lahiri, Observation of preequilibrium emission of neutrons in α -induced reaction on ^{93}Nb , 61st DAE-BRNS Symposium on Nuclear Physics, Saha Institute of Nuclear Physics, Kolkata, December 05-09, 2016.
10. Dibyasree Choudhury, Nabanita Naskar, Susanta Lahiri, Determination of dynamic dissociation constant of clinically important ^{88}Y - and ^{88}Zr - PVP complexes, 14th International Symposium on Metal Ions in Biology and Medicine and 4th Green Health Conference, Mumbai, India, November 28-30, 2016.

11. Nabanita Naskar, Dibyasree Choudhury, Susanta Lahiri, Determination of ^{99}Tc by LSC-TDCR technique, 14th International Symposium on Metal Ions in Biology and Medicine and 4th Green Health Conference, Mumbai, India, November 28-30, 2016.
12. Gairik Mukherjee, Chinmay Saha, Abhishek Mukherjee, Nabanita Naskar, Susanta Lahiri, A. Lahiri Majumder, Anindita Seal, An Endophytic Bacterial Consortium Improves Arsenic Phytoremediation Efficacy of an Arsenic Accumulator *Solanum nigrum*, 14th International Symposium on Metal Ions in Biology and Medicine and 4th Green Health Conference, Mumbai, India, November 28-30, 2016.
13. Kakoli Banerjee, Nabanita Naskar, Dibyasree Choudhury, Susanta Lahiri, Assessment of selected heavy metals in Vermilion (Sindoor) by ICP-OES, 14th International Symposium on Metal Ions in Biology and Medicine and 4th Green Health Conference, Mumbai, India, November 28-30, 2016.
14. Susanta Lahiri, Green synthesis of nano-particles by in situ radiation National Conference on Nanoscience, Nanotechnology and Advanced Materials (NCNNAM-2016), Birla Institute of Technology Mesra, September 26-27, 2016 (**Keynote address**).
15. Susanta Lahiri - Dibyasree Choudhury, Converter Target Chemistry : A new challenge to the Radioanalytical Chemistry – and its relevance with MEDICIS programme, Workshop on Radiochem Aspects of MEDICIS, CERN, Switzerland, September 23, 2016 (**Invited talk**)
16. L. Lens, A. Yakushev, Ch.E. Düllmann, M. Asai, M. Block, H.M. David, J. Despotopulos, A. Di Nitto, K. Eberhardt, M. Götz, S. Götz, H. Haba, L. Harkness-Brennan, F.P. Heßberger, R.-D. Herzberg, D. Hinde, J. Hoffmann, A. Hübner, E. Jäger, D. Judson, J. Khuyagbaatar, B. Kindler, Y. Komori, J. Konki, J.V. Kratz, J. Krier, N. Kurz, M. Laatiaoui, S. Lahiri, B. Lommel, M. Maiti, A.K. Mistry, C. Mokry, K. Moody, Y. Nagame, J.P. Omtvedt, P. Papadakis, V. Pershina, D. Rudolph, J. Runke, M. Schädel, P. Scharrer, T. Sato, D. Shaughnessy, B. Schausten, J. Steiner, P. Thörle-Pospiech, N. Trautmann, K. Tsukada, J. Uusitalo, A. Ward, M. Wegrzecki, E. Williams, N. Wiehl, V. Yakusheva, Single atom flerovium chemistry at TASCA, Ninth International Conference of Nuclear and Radiochemistry (NRC9), Helsinki, Finland, August 29 - September 2, 2016.
17. A. Yakushev, Ch.E. Düllmann, M. Asai, M. Block, H. David, J. Despotopulos, A. Di Nitto, K. Eberhardt, U. Forsberg, P. Golubev, M. Götz, S. Götz, H. Haba, L. Harkness-Brennan, F.P. Heßberger, R.-D. Herzberg, D. Hinde, J. Hoffmann, A. Hübner, E. Jäger, D. Judson, J. Khuyagbaatar, B. Kindler, Y. Komori, J. Konki, J.V. Kratz, J. Krier, N. Kurz, M. Laatiaoui, S. Lahiri, L. Lens, B. Lommel, Ch. Lorentz, M. Maiti, A.K. Mistry, C. Mokry, K. Moody, Y. Nagame, J.P. Omtvedt, P. Papadakis, V. Pershina, D. Rudolph, J. Runke, M. Schädel, P. Scharrer, L.G. Sarmiento, T. Sato, D. Shaughnessy, B. Schausten, J. Steiner, P. Thörle-Pospiech, N. Trautmann, K. Tsukada, J. Uusitalo, A. Ward, M. Wegrzecki, E. Williams, N. Wiehl, V. Yakusheva, Gas Phase Chemistry of Superheavy Elements coupled to an

- electromagnetic separator, Ninth International Conference of Nuclear and Radiochemistry (NRC9), Helsinki, Finland, August 29 - September 2, 2016.
18. Dibyasree choudhury, Nabanita Naskar, Moumita Maiti, Susanta Lahiri, Separation of lead and bismuth from proton irradiated lead-bismuth eutectic by differential precipitation, 99th Canadian Chemistry Conference and Exhibition, Halifax, Canada June 05-09, 2016
 19. Susanta Lahiri, Nabanita Naskar, Punarbasu Chaudhuri, Revisiting NORM measurement, 99th Canadian Chemistry Conference and Exhibition, Halifax, Canada June 05-09, 2016 (**Invited talk**)
 20. Deepak Kumar, Moumita Maiti, Susanta Lahiri, A new method of production and separation of no-carrier-added ⁹⁷Ru from ¹¹B activated natural yttrium target, 7th DAE-BRNS Biennial Symp on Emerging Trends in Separation Science and Technology, SESTEC 2016, Indian Institute of Technology, Guwahati, May 17-20, 2016.
 21. Dibyasree Choudhury, Kaustab Ghosh, Kangkana Sarkar, Nabanita Naskar and Susanta Lahiri, Ionic Liquid-Salt Based Aqueous Biphasic System for Quick Separation of No-Carrier-Added ²⁰³Pb from Proton Irradiated ^{nat}Tl₂CO₃ Target, 7th DAE-BRNS Biennial Symp on Emerging Trends in Separation Science and Technology, SESTEC 2016, Indian Institute of Technology, Guwahati, May 17-20, 2016.
 22. Kangkana Sarkar, Susanta Lahiri, Kamalika Sen, Isolation of Therapeutically Important No-Carrier-Added ²⁰³Pb from Proton Irradiated ^{nat}Tl₂CO₃ using Calcium Alginate Hydrogels, 7th DAE-BRNS Biennial Symp on Emerging Trends in Separation Science and Technology, SESTEC 2016, Indian Institute of Technology, Guwahati, May 17-20, 2016.
 23. Susanta Lahiri, Ride on Time Machine, User interaction workshop on Accelerator Mass Spectrometry dating, IUAC, New Delhi, April 21-23, 2016.
 24. Nabanita Naskar, Susanta Lahiri, Punarbasu Chaudhuri, First report on primordial and anthropogenic radionuclides in indian sundarban mangrove ecosystem, First International Conference on Radioanalytical and Nuclear Chemistry (RANC-2016), Budapest, Hungary, April 10–15, 2016
 25. **Susanta Lahiri**, Moumita Maiti, Dibyasree Choudhury, convertertarget chemistry – a new challenge to the radioanalytical chemistry, First International Conference on Radioanalytical and Nuclear Chemistry (RANC-2016), Budapest, Hungary, April 10–15, 2016 (**Invited talk**).
 26. Susanta Lahiri, The Periodic Table, Recent Advances in Chemistry, scheduled P G Deptt of Chemistry, T M Bhagalpur University, Bhagalpur, February 25-26, 2016 (**Invited talk**)
 27. Susanta Lahiri, The story of triangular affair, National seminar on Design, Synthesis, Interactions, Chemical and Biochemical Activities of Different Functional

Molecules, The University of Burdwan, Burdwan, February 4-16, 2016 (**Invited talk**).

28. Santu Maity, Susanta Lahiri, Jhuma Ganguly, Smart Hydrogel for Rapid and Selective Separation of Long Lived Fission Products: A Greener Approach, 11th International IUPAC Conference on Polymer-Solvent Complexes & Intercalates (POLYSOLVAT-11), Indian Association of Cultivation of Sciences, Kolkata, January 27-30, 2016.
29. Susanta Lahiri, Story of six blind men, National Seminar on Perspectives in Environmental and Marine Research: Retrospect and Prospect, University of Calcutta, January 22, 2016 (**Invited talk**)
30. Susanta Lahiri, Building The Periodic Table – from Marie Curie to today, Fiftysecond Annual Convention of Chemists 2015 and International Conference on Recent Advances in Chemical Sciences, JECRC University, Jaipur December 28-30, 2015 (**Professor J. C. Ghosh Memorial Award Lecture, 2014**).
31. Nabanita Naskar, Susanta Lahiri, Punarbasu Chaudhuri, Assessment of primordial ⁴⁰K in Sundarban area, Fiftysecond Annual Convention of Chemists 2015 and International Conference on Recent Advances in Chemical Sciences, JECRC University, Jaipur December 28-30, 2015.
32. Kangkana Sarakar, Susanta Lahiri, Kamalika Sen, Adsorption of cadmium by microporous calcium alginate beads, Fiftysecond Annual Convention of Chemists 2015 and International Conference on Recent Advances in Chemical Sciences, JECRC University, Jaipur December 28-30, 2015.
33. Moumita Maiti, **Susanta Lahiri**, Zoltan Szucs, S. Takacs, Theoretical estimation on the heavy ion induced production of ¹⁶³Ho: A promising source for direct measurement of neutrino mass, 14th International Conference on Modern Trends in Activation Analysis, MTAA14, Delft University of Technology, Delft, The Netherlands, August 23-28, 2015
34. Nabanita Naskar, **Susanta Lahiri**, Punarbasu Chaudhuri, Alok Srivastava, Anomalies in NORM Measurement, 11th International Conference on Nuclear Analytical Methods in the Life Sciences, NAMLS-11, Delft University of Technology, Delft, The Netherlands, August 23-28, 2015.
35. Kangkana Sarakar, Susanta Lahiri, Kamalika Sen, Calcium alginate and its modification with hesperidin: A separation matrix of no-carrier added lead and thallium, National Symposium on Recent Advances in Chemistry (2015), University of Calcutta, Kolkata, July 31-August 01, 2015.
36. Nabanita Naskar, Susanta Lahiri, Punarbasu Chaudhuri, First-time assessment of primordial radionuclides in the coastal region of Indian Sundarban, National Symposium on Recent Advances in Chemistry (2015), University of Calcutta, Kolkata, July 31-August 01, 2015.

37. Susanta Lahiri, In situ radiation: a powerful tool to synthesize nanoparticles in green method, National Seminar on Research Aspirants of nano materials and its applications, S J C Institute of Technology, Chikballapur, July 21-22, 2015 (**Invited talk and chief guest**)
38. **Susanta Lahiri**, Moumita Maiti, Thierry Stora, Radionuclides in Medicine: from The First Clinical Use of Radium to CERN-MEDICIS, Third International Conference on Radiations and Applications in various fields of research (RAD-2015), Budva, Montenegro, June 8-12, 2015 (**Invited talk**).
39. **Susanta Lahiri**, Moumita Maiti, Radio-Green Chemistry or Green-Radiochemistry?, Third International Conference on Radiations and Applications in various fields of research (RAD-2015), Budva, Montenegro, June 8-12, 2015.
40. Donald Hougbo, Ana-paula Bernardes, Jean-christophe David, Melanie Delonca, Bernadette Hammer, Kalvis Kravalis, **Susanta Lahiri**, Roberto Losito, Cesare Maglioni, Anthony Marchix, Tania Melo Mendonca, Lucia POPESCU, Maria Dorothea SCHUMANN, Paul SCHUURMANS, Thierry Stora, Joachim Vollaire, Jan Vierendeels, International Conference on Electromagnetic Isotope Separators and Related Topics (EMIS), Grand Rapids, Michigan. May 11-15, 2015.
41. Susanta Lahiri, Radiochemistry: Past, Present and Prospects, International Conference on Methods and Applications of Radioanalytical Chemistry (MARC-X), Kona, Hawai'i, USA, April 12-17, 2015 (**Hevesy Medal Presentation talk**).
42. Moumita Maiti, Susanta Lahiri, Zoltán Szűcs, Separation of ^{163}Er from dysprosium target: A step toward neutrino mass measurement through electron capture of ^{163}Ho , International Conference on Methods and Applications of Radioanalytical Chemistry (MARC-X), Kona, Hawai'i, USA, April 12-17, 2015.
43. Kangkana Sarakar, Kamalika Sen, Susanta Lahiri, PVA Based Hydrogels for Uranium (VI) Pre-concentration: An Attempt to Separate ^{226}Ra from Bulk Uranium, Theoretical Chemistry, Synthesis, Reactivity and Structure Evaluation, University of Burdwan, February 19-21, 2015.
44. Susanta Lahiri, A Ride on Time Machine, Advanced Spectroscopy, Theoretical Chemistry, Synthesis, Reactivity and Structure Evaluation, University of Burdwan, February 19-21, 2015. (**Invited talk**)
45. Kaustab Ghosh, Moumita Maiti, Susanta Lahiri, Radiochemical separation of $^{195\text{(m,g)},197\text{m}}\text{Hg}$ from gold target using RTIL 1-butyl-3-methylimidazolium hexafluorophosphate, Nuclear and Radiochemistry Symposium (NUCAR-2015), Bhabha Atomic Research Centre, Trombay, Mumbai, February 9-13, 2015.
46. Santu Maity, Arpita Datta, Susanta Lahiri, Jhuma Ganguly, Synthesis of New Greener Biopolymer Chitosan Based Hydrogel and Its Application for Separation of ^{152}Eu and ^{137}Cs , Nuclear and Radiochemistry Symposium (NUCAR-2015), Bhabha Atomic Research Centre, Trombay, Mumbai, February 9-13, 2015.

47. Moumita Maiti, Arpita Datta, Susanta Lahiri, Aqueous Biphasic Separation of ^{97}Ru and $^{95,96}\text{Tc}$ from Yttrium, Nuclear and Radiochemistry Symposium (NUCAR-2015), Bhabha Atomic Research Centre, Trombay, Mumbai, February 9-13, 2015.
48. Arpita Datta, Moumita Maiti, Susanta Lahiri, Search for a New Greener Technology for Separation of NCA ^{97}Ru from Bulk Nb: Ionic Liquid Based Aqueous Biphasic System, Nuclear and Radiochemistry Symposium (NUCAR-2015), Bhabha Atomic Research Centre, Trombay, Mumbai, February 9-13, 2015.
49. Moumita Maiti, **Susanta Lahiri**, Is Classical Chemistry Relevant for Converter Targets? ISOLDE workshop and users meeting 2014, 50th Anniversary Edition, CERN, Switzerland, December 14-17, 2014.
50. Moumita Maiti, Susanta Lahiri, A long way to confirm element 117, Workshop on Science with Rare Ion Beams (SCRIBE-2014), VECC Kolkata, November 25-28, 2014.
51. Z. Szucs, B. Kovacs, R. Doczi, M. Maiti, Susanta Lahiri, Automated Unit for separation of arsenic by iron doped calcium alginate, 5th International Congress on Arsenic in the Environment (As2014), Buenos Aires, Argentina, May 11-16, 2014.
52. A.P. Bernardes, J.C. David, S. Lahiri, M. Maiti, A Marchix, T. Melo Mendonça, T. Stora, Radiological inventory assessment for a compact loop made of molten lead-bismuth eutectic (LIEBE project at CERN-ISOLDE facility), Twelfth Meeting of Task-Force on Shielding Aspects of Accelerators, Targets and Irradiation Facilities, *Fermilab*, USA, 28-30 April 2014
53. Kaustab Ghosh, Moumita Maiti, Susanta Lahiri, Separation of no-carrier added ^{62}Zn from ^7Li irradiated cobalt target using calcium alginate beads, Nuclear Analytical Chemistry (NAC-5), Bhabha Atomic Research Centre, Mumbai, January 20-24, 2014
54. Kaushik Gangopadhyay, Moumita Maiti, Susanta Lahiri, Prediction on the origin of ancient glass beads by studying its potassium content by Compton Suppressed γ -ray Spectrometry, Fifth Symposium on Nuclear Analytical Chemistry (NAC-5), Bhabha Atomic Research Centre, Mumbai, January 20-24, 2014 (**Invited talk**).
55. Kaustab Ghosh, V. Afzal Hussain, Moumita Maiti, Susanta Lahiri, Ionic Liquid-Salt Based Aqueous Biphasic System for Separation of ^{109}Cd from Silver Target, Third International Conference on Application of Radiotracers and Energetic Beams (ARCEBS-14), Ffort Raichak, Kolkata January 12-18, 2014
56. Zoltán Szűcs, Sándor Takács, Moumita Maiti, Susanta Lahiri, Production of ^{163}Ho Radioisotope via Indirect Nuclear Reaction by Proton and Deuteron: Comparison of Theoretical Calculation and Experimental Data, Third International Conference on Application of Radiotracers and Energetic Beams (ARCEBS-14), Ffort Raichak, Kolkata January 12-18, 2014.
57. Moumita Maiti, Kaustab Ghosh, T.M. Mendonça, Thierry Stora, Susanta Lahiri, First Experiment on Production of Radionuclides in 1.4 GeV Proton Induced Reaction on

- Thick LBE Target, Third International Conference on Application of RadiotraCers and Energetic Beams (ARCEBS-14), Ffort Raichak, Kolkata January 12-18, 2014
58. Arpita Datta, Moumita Maiti, Susanta Lahiri, Separation of ^{97}Ru from Niobium Target Using PEG Based Aqueous Biphasic Systems, Third International Conference on Application of RadiotraCers and Energetic Beams (ARCEBS-14), Ffort Raichak, Kolkata January 12-18, 2014
 59. Ajoy Mandal, Moumita Maiti, Ranak Das, Susanta Lahiri, Determination of Potassium in Common Vegetables Using Compton Suppressed Gamma Spectroscopy, Third International Conference on Application of RadiotraCers and Energetic Beams (ARCEBS-14), Ffort Raichak, Kolkata January 12-18, 2014
 60. Susanta Lahiri, Moumita Maiti, Kaustab Ghosh, Tania Manuela De Melo Mendonca, Thierry Stora, First report on the inventory of radionuclides in 1.4 GeV proton irradiated thick lead-bismuth (LBE) target, ISOLDE Physics Workshop and Users Meeting, CERN, Switzerland, November 25-27 (2013).
 61. Moumita Maiti, Susanta Lahiri, Generation of Nuclear data for the production of ^{97}Ru from $^{12}\text{C}+^{89}\text{Y}$ reaction, 5th Asia Pacific Symposium on Radiochemistry (APSORC-13), Kanazawa, Japan, September 22-27 (2013) (**Invited talk**).
 62. Ajoy Mandal, Kaustab Ghosh, Moumita Maiti, Susanta Lahiri, Studies on As and Se uptake by Mung Bean, Fifth International Congress of the Federation of the European Societies for Trace Elements and Minerals, Avignon, France, May 22-24, 2013.
 63. **Susanta Lahiri**, An New Non-destructive Method of Potassium Determination in Food One day conference on Food, Debrecen University, Hungary, April 04, 2013 (**Keynote address**)
 64. Susanta Lahiri, ICP-state of the art instruments for trace analysis, Thematic Workshop on Trace Element analysis and Radiological Sciences, Manipur University, Imphal, 12-14 March 2013 (**Invited talk**).
 65. Susanta Lahiri and Moumita Maiti, Nutrino mass measurement and radiochemistry, Nuclear and Radiochemistry Symposium, NUCAR-2013, R.D. University, Jabalpur, February 19-23, 2013 (**Invited talk**).
 66. Kaustab Ghosh, Moumita Maiti and Susanta Lahiri, "Role of RTIL 1 butyl-3-methylimidazolium hexafluorophosphate in separation of no-carrier-added ^{109}Cd from alpha-particle irradiated natural silver target" Nuclear and Radiochemistry Symposium, NUCAR-2013, R.D. University, Jabalpur, February 19-23, 2013.
 67. Moumita Maiti and Susanta Lahiri, "Nuclear and chemical data towards the production of no-carrier-added ^{97}Ru radionuclides from natural yttrium target" Nuclear and Radiochemistry Symposium, NUCAR-2013, R.D. University, Jabalpur, February 19-23, 2013.
 68. Susanta Lahiri, Moumita Maiti, ZoltánSzűcs and Sandor Takacs, Alternative production routes and new separation methods for no-carrier-added ^{163}Ho , The

Future of Neutrino Mass Measurements: Terrestrial, Astrophysical and Cosmological Measurements in the next decade (vMass13), Milano, Italy 4-7 February 2013 **(Invited talk)**.

69. Susanta Lahiri, Moumita Maiti, ZoltánSzűcs, Sandor Takacs, ^{163}Ho , Collaboration meeting on Electron Capture Holmium Neutrino (ECHO), Johannes Gutenberg Universitat Mainz, January 21, 2013 **(Invited talk)**
70. Susanta Lahiri, Biomonitoring, Last 100 Year's of Science in India: Satellite Programme, Saha Institute of Nuclear Physics, Kolkata, January 09-10, 2013 **(Invited talk)**
71. Binita Dutta, Susanta Lahiri, B.S.Tomar, Separation of no-carrier-added rhenium from bulk tantalum by citrate salt based aqueous biphasic system, Acharya Prafulla Chandra Ray Memorial Symposium on Chemistry and Industry (2012), The Indian Chemical Society, Kolkata, August 02-03, 2012.
72. Susanta Lahiri, Chemistry of Lead Bismuth Loop, Kick off meeting for lead bismuth loop, CERN, Switzerland, May 10, 2012. **(Invited talk)**
73. Susanta Lahiri, Chemistry of Lead Bismuth Loop, International workshop on Future plan with radioactive beam, Saha Institute of Nuclear Physics, India, April 16-18, 2012. **(Invited talk)**
74. Susanta Lahiri; Moumita Maiti, Chromatographic separation of no-carrier-added ^{97}Ru from ^{12}C irradiated natural yttrium target, Methods & Application of Radioanalytical Chemistry (MARC-IX), March 25-30, 2012, USA.
75. Kaustab Ghosh, Moumita Maiti, Susanta Lahiri, One step chromatographic separation of ^{111}In , ^{109}Cd from alpha particle induced silver target, Emerging Trends in Separation Science and Technology (SESTEC-2012), VKM's Mithibai College, Mumbai 400056, February 27 - March 01, 2012.
76. Swadesh Mandal, Ajoy Mandal, Susanta Lahiri, Speciation dependent extraction studies of ^{99}Mo and $^{99\text{m}}\text{Tc}$ and their separation from their equilibrium mixture, Emerging Trends in Separation Science and Technology (SESTEC-2012), VKM's Mithibai College, Mumbai 400056, February 27 - March 01, 2012.
77. Binita Dutta, Susanta Lahiri, B.S. Tomar, A novel environmentally benign approach for separation of no-carrier-added rhenium from bulk tantalum by sodium malonate-PEG aqueous biphasic system, Emerging Trends in Separation Science and Technology (SESTEC-2012), VKM's Mithibai College, Mumbai 400056, February 27 - March 01, 2012.
78. Binita Dutta, Susanta Lahiri, B.S. Tomar, Separation of no-carrier-added rhenium from bulk tantalum by precipitation technique, Emerging Trends in Separation Science and Technology (SESTEC-2012), VKM's Mithibai College, Mumbai 400056, February 27 - March 01, 2012.

79. Ajoy Mandal and Susanta Lahiri, Radiochemical separation of no-carrier-added As and Se from ^7Li irradiated germanium oxide target, Emerging Trends in Separation Science and Technology (SESTEC-2012), VKM's Mithibai College, Mumbai 400056, February 27 - March 01, 2012.
80. Susanta Lahiri, In situ γ -radiation: an unique and environmentally benign tool for nano particle synthesis, International conference on "Frontiers in Nanoscience, Nanotechnology and their Applications (NanoSciTech-2012), February 15-18, 2012, Panjab University, Chandigarh, India (**Invited talk**)
81. Susanta Lahiri, Search of new elements after Madam Curie, National Seminar on Modern Trends of Chemistry in 21st Century, February 6-7, 2012, St. Paul's College, Kolkata, India (**Invited talk**)
82. S. Lahiri, M. Maiti, K. Ghosh, Production and separation of ^{111}In : an important radionuclide in life sciences, Tenth International Conference on Nuclear Analytical Methods in the Life Sciences (NAMLS-10), 15-20 January, 2012, Bangkok, Thailand (**Invited talk**)
83. Z. Szucs, S. Takács, M. Maiti, S. Lahiri, Production of ^{75}Se for tracking of radiochemical separation of ^{79}Se from radioactive waste of nuclear power plant, Tenth International Conference on Nuclear Analytical Methods in the Life Sciences (NAMLS-10), 15-20 January, 2012, Bangkok, Thailand.
84. Binita Dutta, Susanta Lahiri, B.S. Tomar, Aqueous biphasic separation of no-carrier-added rhenium from bulk tantalum target, Tenth International Conference on Nuclear Analytical Methods in the Life Sciences (NAMLS-10), 15-20 January, 2012, Bangkok, Thailand.
85. M. Maiti, K. Ghosh, S. Lahiri, A green approach for the separation of no-carrier-added ^{111}In , ^{109}Cd from alpha particle activated natural silver target, Tenth International Conference on Nuclear Analytical Methods in the Life Sciences (NAMLS-10), 15-20 January, 2012, Bangkok, Thailand.
86. Banhi Chatterjee, Abhijit Bisoi, Dibyadyuti Pramanik, Sudatta Ray, Aditya Priyant, Maitreyee Saha Sarkar, Maitreyee Nandy*, "Environmental Radioactivity Analysis at Kolkata after Fukushima Accident" 12th International Conference on Radiation Shielding (**ICRS-12**), Atomic Energy Society of Japan, Nara, Japan, September 2nd - 7th, 2012.
87. Maitreyee Nandy "Induced Activity in Tungsten as An ADSS Target", 12th International Conference on Radiation Shielding (**ICRS-12**), Atomic Energy Society of Japan, Nara, Japan, September 2nd - 7th, 2012.

Biodata (2012-2016)



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EDUCATION

1986: Ph.D. in Chemistry, Calcutta University (SINP)

1979: M.Sc. in Chemistry, University of Calcutta

1976: B.Sc. Chemistry Hons, University of Calcutta

ACADEMIC POSITIONS

2015- : Senior Professor H (presently in extension period), Saha Institute of Nuclear Physics

2007-2014: Professor G, Saha Institute of Nuclear Physics

2003-2007: Professor F, Saha Institute of Nuclear Physics

1999-2003: Associate Professor E, Saha Institute of Nuclear Physics

1995-1999: Reader D, Saha Institute of Nuclear Physics

1992-1995: Lecturer C, Saha Institute of Nuclear Physics

AWARDS/ HONOURS

Received the SINP Silver Medal during Diamond Jubilee Celebration in January 2010 as the co-author of the highest Cited article of the Institute

PUBLICATIONS (2012-2016): Cumulative impact Factor 61.685

1. Polypyrrole – Titanium(IV) doped Iron(III) oxide Nanocomposites: Synthesis, Characterization with Tunable Electrical and Electrochemical Properties, Debabrata Nandi, Arup Kumar Ghosh, Amitabha De, Pintu Sen, Kaushik Gupta, Ankan Dutta Chowdhury and Uday Chand Ghosh, **Materials Research Bulletin** 47 (2012) 2095–2103. I.F. 2.105

2. Label Free Polyaniline Based Impedimetric Biosensor for Detection of E. coli O157:H7 Bacteria, Ankan Dutta Chowdhury; Amitabha De, Chiroree Roy Chaudhuri;

Krishnan Bandyopadhyay; Pintu Sen, **Sensors and Actuators B** 171– 172 (2012) 916–923. I.F. 4.582

3. Functionalized Polyaniline Nanowires for Biosensing, RupaliGangopadhyay; Ankan Dutta Choudhury; Amitabha De, **Sensors and Actuators B** 171– 172 (2012) 777– 785. I.F. 4.582

4. Manganese incorporated iron(III) oxide- graphene magnetic nanocomposite: Synthesis, characterization and application for the arsenic(III)-sorption from aqueous solution, Debabrata Nandi, Arup Kumar Ghosh, Amitabha De, Pintu Sen, Kaushik Gupta and Uday Chand Ghosh, **Journal of Nanoparticle Research** Volume: 14 Issue: 12 Article Number: 1272 Dec. 2012. I.F. 3.287

5. Thermally stable polypyrrole- Mn doped Fe(III) oxide nanocomposite sandwiched in graphene layer: synthesis, characterization with tunable electrical conductivity Debabrata Nandi, Kaushik Gupta, Arup Kumar Ghosh, Amitabha De, NiharRanjan Ray and Uday Chand Ghosh. **Chemical Engineering Journal** Volume: 220 Pages: 107-116 March 15, 2013. I.F.5.439

6. Reduced Graphene Oxide/ Ethylene Vinyl Acetate Co-polymer Composite with Improved Thermal Stability and Flame Retardancy: Debabrata Nandi, Atanu Talukdar, Uday Chand Ghosh, Amitabha De, Satyaban Bhunia and Arup Kumar Ghosh **J. Polym. Mater.** Vol. 29, No. 4, 2012, 401-411. I.F. 1.204

7. [Functionalised Polyaniline Nanowires: A Prospective Biosensing Platform](#) Gangopadhyay, Rupali; Chowdhury, Ankan Dutta; De, Amitabha **Asian Journal of Chemistry** Volume: 25 Supplement: S Pages: S369-S372 Published: 2013. I.F. 0.253

8. Conducting Polymer based Manganese Dioxide Nanocomposite as Supercapacitor Pintu Sen, Amitabha De, Ankan Dutta Chowdhury, S.K. Bandyopadhyay, Nidhi Agnihotri and M. Mukherjee **Electrochimica Acta** 108 (2013) 265– 273. I.F. 4.721

9. Highly sensitive electrochemical biosensor for Glucose, DNA and Protein using Gold-Polyaniline Nanocomposites as a common matrix. Ankan Dutta Chowdhury, RupaliGangopadhyay and Amitabha De; **Sensors and Actuators B** 190 (2014) 348–356. I.F. 4.582

10. Mechanistic Insight for Sorption of Cd(II) and Cu(II) from Their Aqueous Solution on Magnetic Mn-Doped Fe(III) Oxide Nanoparticles Implanted Graphene. Nandi, Debabrata; Basu, Tina; Debnath, Sushanta; Ghosh, Arup; De, Amitabha; Ghosh, Uday **Journal of Chemical & Engineering Data**, Volume 58, issue 10 (October 10, 2013), p. 2809-2818. I.F. 2.004

11. Fabrication, nanostructure evaluation, 3D electrical transport and electrochemical capacitance of PEDOT - Ti(IV) doped iron(III) oxide nanocomposite. Debabrata Nandi,

Arup K. Ghosh, Amitabha De, Pintu Sen and Uday Chand Ghosh; **J. Mater. Sci.** (2014), 49, 776-785. I.F. 2.163

12. Conducting CoMn_2O_4 - PEDOT nanocomposites as catalyst in oxygen reduction reaction. Ankan Dutta Chowdhury, Nidhi Agnihotri, Pintu Sen, Amitabha De; **Electrochimica Acta**, [Volume 118](#), 1 February 2014, Pages 81–87. I.F. 4.721

13. Polypyrrole decorated graphene nanostructure: Fabrication, depiction and anomalous dimensional crossover in electronic conduction. Debabrata Nandi, Prasun K. Pal, Arup K. Ghosh, Amitabha De, Uday Chand Ghosh; **Applied Surface Science** 293 (2014) 90–96. I.F. 2.11

14. Positional effect of single base mismatch in DNA: Enhanced detection by electrochemical method. Ankan Dutta Chowdhury, Nidhi Agnihotri, Amitabha De and Munna Sarkar; **Sensors and Actuators B** 202 (2014) 917–923. I.F. 4.582

15. Non-Enzymatic Electrochemical Detection of Cholesterol using β -Cyclodextrin Functionalized Graphene Nidhi Agnihotri, Ankan Dutta Chowdhury, Amitabha De **Biosensors and Bioelectronics** 63 (2015) 212-217. I.F. 7.476

16. Hydrolysis of sodium borohydride using Ru–Co-PEDOT nanocomposites as catalyst Ankan Dutta Chowdhury, Nidhi Agnihotri, Amitabha De **Chemical Engineering Journal** 264 (2015) 531–537. I.F. 5.439

17. Hierarchically designed PEDOT encapsulated Graphene- MnO_2 nanocomposite as Supercapacitors Nidhi Agnihotri, Pintu Sen, Amitabha De and Manabendra Mukherjee **Materials Research Bulletin** 88 (2017) 218-225. I.F. 2.435

GUIDANCE/TEACHING

Ph.D. degree awarded: 5 [in the period 2012-2016: 2]; Thesis submitted: 1
Summer Project Student: 5

NATIONAL/INTERNATIONAL CONFERENCES

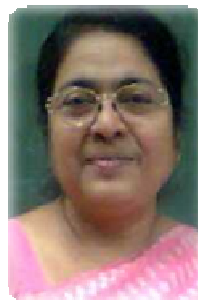
Invited Talk: 8 (India:6; Overseas:2)

RESEARCH AND DEVELOPMENT

Highlights of research activity during 2012-16 was mainly concentrated on the application of conducting polymers and their nanostructured composite materials and graphene based materials for fabricating biosensors for different biomolecules and energy storage devices like supercapacitors, hydrogen generation etc.

Important achievements are following : Fabrication of electrochemical biosensors for DNA and glucose sensing and label free impedimetric biosensor E. Coli O157; H7 using Gold nanoparticles (AuNP) incorporated Polyaniline nanowires (PAN-NW). A novel non-enzymatic approach towards cholesterol detection is achieved, exploiting the

electrochemical route of sensing which has a distinct advantage over other conventional enzymatic processes. Chemically converted Graphene modified with β -CD, being hydrophilic, electroactive and high surface area material, provides a platform for the electrochemical detection of Cholesterol using Methelene Blue. Hierarchically designed binary composite Grp-MnO₂ and ternary nanocomposite of PEDOT:Grp-MnO₂ was synthesized as electrode materials for high performance supercapacitors.. Supercapacitive behaviour of the nanocomposites was tested and established using them as electrodes for electrochemical studies like cyclic voltammetry and charge-discharge. Highest specific capacitance value was found to be 213 Fg⁻¹ for the PEDOT:Grp-MnO₂ with improved energy and power densities. Development of easy, facile and rapid synthetic methodologies for producing highly active low-cost bifunctional electrocatalysts PEDOT-CoMnO₄ nanocomposite for 4e⁻ oxygen reduction/evolution reactions (ORR/OER) which are the key barriers in various electrochemical devices such as metal–air batteries, fuel cells and water splitting reaction. Graphite nanoplatelet (GNP)/conducting polymer (PEDOT:PSS) composites were synthesized to evaluate the electromagnetic interference (EMI) shielding effectiveness (SE) in the X-band frequency region. Owing to their low density, GNP/ PEDOT:PSS composites give high specific EMI SE up to 67.3 dB.cm³/g, which is higher compared to even foam structures particularly designed for making low density EMI shields.



SAMITA BASU, Sr. Professor H+

DoB 01 January 1959

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EDUCATION

1989: Ph.D. in Chemistry, Jadavpur University (Indian Association for the Cultivation of Science, Jadavpur, Kolkata)

1982: M.Sc. in Chemistry, University of Calcutta (Batch Year: 1980)

1979: B.Sc. Chemistry Hons, University of Calcutta (Batch Year: 1978)

ACADEMIC POSITIONS

2016- : Senior Professor H+, Saha Institute of Nuclear Physics

2013-2016: Professor H, Saha Institute of Nuclear Physics

2007-2013: Professor G, Saha Institute of Nuclear Physics

2002-2007: Professor F, Saha Institute of Nuclear Physics

1998-2002: Associate Professor E, Saha Institute of Nuclear Physics

1994-1998: Reader D, Saha Institute of Nuclear Physics

1992-1994: Lecturer C, Saha Institute of Nuclear Physics

AWARDS/ HONOURS

Professor P.K. Bose Memorial Award, Indian Chemical Society, 2012

Foundation Day Award for the year 2010 at Saha Institute of Nuclear Physics, Kolkata

Member of International Spin Chemistry Committee from 2005

Fellow of the West Bengal Academy of Science and Technology in the year 2010 for contributions in the field of Molecular Spectroscopy and Executive Committee member during 2013 - 2016

Member of Academic Advisory Board, Jagadis Bose National Science Talent Search (JBNSTS) Kolkata, from 2008

Member of Board of Studies of the Department of Microbiology of St. Xavier's College (Autonomous), Kolkata, from 2010

Professor, Homi Bhabha National Institute, BARC, Mumbai from 2013

Reviewer of papers submitted in peer-reviewed International Journals (ACS, Elsevier, RSC, Springer, Willey, etc)

Examiner of Ph. D. Thesis & viva voce examinations of NEHU, IIT Kharagpur, JNTU Hyderabad, Visva-Bharati, Manipur University, Burdwan University, Calcutta University, Jadavpur University, etc during 2012-16.

Members of National Advisory Committee of conferences, RDPAP-2016, Sambalpur; RAMS-2016, Hyderabad; UFS-2015, Kolkata; LCMB-2014, IIT Kharagpur; etc.

PUBLICATION STATISTICS

Journals: 135 (for 2012-2017: 39; I.F. = 117.591 (Average: 3.015); citation = 216); Chapter of Books: 4 (for 2012-2016: 2); *h*-index: 18

SELECTED PUBLICATIONS (2012-2016)

Book Chapter: Research Methodology in Chemical Sciences Experimental and Theoretical Approach; Editors: Tanmoy Chakraborty & Lalita Ledwani, Apple Academic Press (AAP), USA
Pub Date: August, 2015 **Hard ISBN:** 9781771881272 **Chapter 1:** Magnetic Field Effect on Photo-Induced Interactions: Its Implications in Distance Dependent Photo-Induced Electron Transfer Between CT-DNA and Metal Complex, B Koley Seth and **S. Basu**, page 1-15.

Book Chapter: Computational and Experimental Chemistry: Developments and applications; Editors: Tanmoy Chakraborty, PhD, Michael J. Bucknum, PhD, Eduardo A. Castro, PhD, Apple Academic Press, Toronto & New Jersey and CRC Press Taylor & Francis Group, 2014, "Distance Dependence of Magnetic Field Effect Inside the Confined Heterogeneous Environment: A Case Study with Acridine and N, N-Dimethyl Aniline Inside AOT Reverse Micelles" by M. K. Sarangi and S. Basu, 127-143.

A.Sau, K. Bera, P. Mondal, B. Satpati and **S. Basu**, "Distance-dependent Electron Transfer in Chemically Engineered Carbon Dots", Journal of Physical Chemistry C, 120, 26630-26636, 2016.

[K. Bera](#), [A. Sau](#), [P. Mondal](#), [R. Mukherjee](#), [D. Mookherjee](#), [A. Metya](#), [A. K. Kundu](#), [D. Mandal](#), [B. Satpati](#), [O. Chakrabarti](#) and **S. Basu**, "Metamorphosis of Ruthenium-Doped Carbon Dots: In Search of the Origin of Photoluminescence and Beyond", ACS ChemMater., 28, 7404-7413, 2016.

C. Sengupta and **S. Basu**, "A spectroscopic study to decipher the mode of interaction of some common acridine derivatives with CT DNA within nanosecond and femtosecond time domains", RSC Advances, 5, 78160 - 78171, 2015.

B. Koley Seth, A. Ray, S. Biswas and **S. Basu**, "NiII-Schiff base complex as an enzyme inhibitor of hen egg white lysozyme: a crystallographic and spectroscopic study", Metallomics, 6, 1737—1747, 2014.

P. Mitra, P. K. Chakraborty, P. Saha, P. Ray and **S. Basu**, "Antibacterial efficacy of acridine derivatives conjugated with gold nanoparticles", International Journal of Pharmaceutics, 473, 636-643, 2014.

B. Koley Seth, A. Ray, A. Saha, P. Saha, **S. Basu**, "Potency of photoinduced electron transfer and antioxidant efficacy of pyrrole and pyridine based Cu(II)-Schiff complexes while binding with CT-DNA", J. Photochem. Photobiol. B, 132, 72-84, 2014.

P. Mitra, B. Chakraborty, D. Bhattacharyya, **S. Basu**, "Excimer of 9-aminocridine hydrochloride hydrate in confined medium: an integrated experimental and theoretical study", J. Phys. Chem. A, 117, 1428-38, 2013.

M. K. Sarangi, A. K. Mitra, C. Sengupta, S. Ghosh, S. Chakraborty, C. Saha, **S. Basu**, Hydrogen Bond Sensitive Probe 5-Methoxy-1-keto-1,2,3,4-tetrahydro Carbazole in the Microheterogeneity of Binary Mixtures and Reverse Micelles”, *J. Phys. Chem. C*, *117*, 2166-2174, 2013.

M. K. Sarangi, A. Mitra, **S. Basu**, “[Prototropic Interactions of Pyrimidine Nucleic Acid Bases with Acridine: A Spectroscopic Investigation](#)”, *J. Phys. Chem. B*, *34*, 10275–10282, 2012

M. K. Sarangi, D. Bhattacharyya, **S. Basu**, “Influence of 2’deoxy sugar moiety on excited state proton equilibrium of Adenine and Adenosine with Acridine inside SDS micelles; A time-resolved study with quantum-chemical calculations”, *Chem. Phys. Chem.*, *13*, 525-534, 2012.

GUIDANCE/TEACHING

Ph.D. degree awarded: 14 [in the period 2012-2017: 7]; Thesis submitted: 1

Research Fellow:1 (continuing); Project (Summer) students (2012-16): 31

Post M.Sc. Biophysical Science: Spectroscopy & Photochemistry

Calcutta University – Department of Inorganic Chemistry M.Sc (Honorary): Spectroscopy

Bidhanagar College, Kolkata M.Sc (Honorary): Photochemistry

Midnapore College, West Bengal M.Sc. (Honorary): Spectroscopy

National/International Conferences

Invited Talk : 44 (India:42; Overseas:2); Organized: 1, Chairperson (only): 1

Research and Development

Area(s) of research: Photophysical and photochemical studies on inter- and intramolecular electron/proton transfer and hydrogen abstraction reactions with small chemically and biologically important molecules and interactions of small drug-like molecules with proteins and DNA bases in homogeneous and heterogeneous confined media as well as with carbon nanodots using steady-state and time-resolved (10^{-9} – 10^{-6}) second spectroscopic techniques, magnetic field effects and X-Ray Crystallography as well as theoretical docking and microscopic (TEM & Superresolution confocal) studies. The metamorphosis of carbon dots is monitored by characterizing each trapped intermediate using HR-TEM, DLS, XPS, XRD, $^1\text{H-NMR}$ and FT-IR.

Highlights of scientific contribution: Simple experiments have been designed to unravel some of the physical aspects, mainly the role of structure of participating molecules and the solvent matrix, in above mentioned reactions. In keeping with current interest in drug-DNA and drug-protein interactions, studies have been extended from small organic molecules to some model biomolecules. Although steady-state and time-resolved absorption and fluorescence help to identify steady-state products and transient intermediates respectively, the importance of magnetic field effect lies in its ability to identify initial spin state, one of the deciding factors for ultimate products, as well as to assess the intermediate distance in geminate spin-correlated radical ion pairs/radical pairs produced as transients, which is very much useful to study ‘distance-dependent’ interactions in biomacromolecules. Very recently we have succeeded in synthesizing ‘photoluminescent’ carbon dots. As per our concern, this is a pioneering work, where the plausible molecular structure and the intrinsic mechanisms governing photoluminescence of carbon dots are explained by trapping seven visibly distinct coloured intermediates.

The photoinduced electron transfer ability of such carbon dots helps to develop their utility as quinone-sensor in live cells.

Development: We have installed MAI TAI HP Laser and accessories (F/5034/C/CSD/SB/CBAUNP) and Femtosecond optically gated fluorescence kinetic measurement system FOG 100-DX (F/5035/C/CSD/SB/CBAUNP) procured from M/s. Newport Corporation and M/s CDP system Corporation respectively in **February, 2014** after renovating the room (No. 232, CSD) to make it dust-free with proper air conditioning, electrical wiring and installing UPS facilities procured from Biomolecular Assembly, Recognition and Dynamics (BARD) project.

Future Research/development

Carbon dots belong to a new class of carbon cluster with high fluorescence quantum yield and can provide useful optical and electronic properties associated with their nanoscale structures. These are nontoxic and their surface functionalities can be easily tuned chemically to use as drug carrier. We like to synthesize different carbon dots using different dopant which would influence their photoluminescent property and generate high fluorescence quantum yield. We like to investigate their interactions with drugs, DNA and model proteins using ultrafast spectroscopy to have detailed mechanisms required for their applications as sensors for selective and controlled drug release in cancer cells.

SUSANTA LAHIRI, Senior Professor H+

Dob 1st August 1961

Phone 9433988997(extn 1118)

Email susanta.lahiri@saha.ac.in



EDUCATION

2009: D.Sc, University of Calcutta

1994: Ph.D. in Chemistry, University of Calcutta

1987: M.Sc. in Chemistry, Burdwan University

ACADEMIC POSITIONS

01.07.2016 – till date,	Senior. Professor H+, SINP
01.01.2013 – 30.06.2016	Senior Professor H, SINP
01.08.2007 - 31.12.2012	Professor-G, SINP
01.08.2004-31.7.2007	Professor-F, SINP
01.08.2000-31.7.2004	Associate Professor E, SINP
03.10.1997-31.7.2000	Reader D, SINP
24.08.1994-02.10.1997	Lecturer, University of Burdwan

AWARDS/HONOURS

- **Hevesy Medal Award 2015** (The **highest international honour** in the field of Nuclear and Radiochemistry). The award was instituted in 1968, after the demise of Nobel Laureate George de Hevesy in 1966. **For the first time someone from India received this award in its history of ~50 years.** (For more details, please see <http://www.thehindu.com/sci-tech/science/susanta-lahiri-cocreator-of-element-117-gets-hevesy-medal/article7105903.ece>).
- **Professor J. C. Ghosh Memorial Award for the year 2014** by Indian Chemical Society.
- **Foundation day Prize** of Saha Institute of Nuclear Physics on January 11, 2012.
- **Selected** in the nine member **“Hevesy Medal Award Selection Panel -2016”** by International Committee for Activation Analysis (First time from India)
- Associate Membership **of the Third World Academy of Sciences (TWAS)** in Centre of Excellence at South (Consequitively two times, 2000-2003, 2004-2006).
- **Tarun Datta Memorial Award '96** (awarded by Indian Association of Nuclear Chemists and Allied Scientists, IANCAS) for excellent research work in the field of Radioanalytical and Nuclear Chemistry in INDIA (bellow 35 years). **Our paper** on

element 117 (published along with international team of scientists) became in the list of “Top Ten Physics News Stories in 2014” as declared by APS.

- **Member**, Editorial Advisory Board, Radiochimica Acta (from 2016)
- **Member** Hevesy Medal Laureate Board, JRNC (since 2015)
- **Member** of Distinguished Reviewers Board of Journal of Radioanalytical and Nuclear Chemistry (since 2005, selected 5 times)
- **Member**, CERN-MEDICIS programme (only member outside Europe)
- **Task group leader (Radiochemistry)**, CERN-ISOLDE, CERN, Geneva
- **Visiting Scientist** – CERN ISOLDE.
- **Member** of International Board of Biomonitoring (IBB) since 2006 (Only member from India in seven member board) (since 2005).
- Guest Editor, Special issue of “Science and Culture” vol 81 (2015)
- Guest Editor, J. Radioanal. and Nuclear Chemistry, vol. 302 (2014)
- Guest Editor, Radiochimica Acta, vol. 100 (2012).
- **Member, International Advisory Board** of prestigious international conferences (below list from 2012):
 - 14th International Symposium on Metal Ions in Biology and Medicine and 4th Green Health Conference, Mumbai, India, November 28-30, 2016, etc.
 - 1st International conference on Radioanalytical and Nuclear Chemistry (RANC-2016), Budapest, Hungary, April 10-16, 2016
 - 5th Asia Pacific Symposium on Radiochemistry’13 (APSORC-13), September 22- 27, 2013 Kanazawa, Japan
 - International Conference on Nuclear and Radiochemistry (NRC-8), Lake Como, Italy, September 16-21, 2012
- **Session Chaired** in many International and National Conferences (list from 2012):
 - Eruption of Radionuclides in Imaging and Therapy, February 25-26, 2017, Kolkata
 - 13th DAE-BRNS Nuclear and Radiochemistry Symposium (NUCAR-2017)
 - International Symposium on Metal Ions in Biology and Medicine and 4th Green Health Conference, Mumbai, India, November 28-30, 2016
 - 7th DAE-BRNS Biennial Symp on Emerging Trends in Separation Science and Technology, SESTEC 2016, Indian Institute of Technology, Guwahati, May 17-20, 2016
 - 1st International conference on Radioanalytical and Nuclear Chemistry (RANC-2016), Budapest, Hungary, April 10-16, 2016
 - International Conference on Modern Trends in Activation Analysis, MTAA14, Delft University of Technology, Delft, The Netherlands, August 23-28, 2015

- National Seminar on Research Aspirants of nanomaterials and its applications, S J C Institute of Technology, Chikballapur, July 21-22, 2015
 - Third International Conference on Radiations and Applications in various fields of research (RAD-2015), Budva, Montenegro, June 8-12, 2015
 - Workshop on Science with Rare Ion Beams (SCRIBE-2014), VECC Kolkata, November 25-28, 2014
 - DAE Nuclear and Radiochemistry Symposium (NUCAR-13), Jabalpur, 19-23 February, 2013
 - And more
- Member, Ph. D Committee, Calcutta University (since 2000), Board of Research Studies, University of Burdwan, Department of Chemistry (since 2015) and School Board of Physical Sciences, Mizoram University, Aizawal.
- I was invited to deliver series of lectures on Green Chemistry to the Ph. D students of University of Debrecen. Hungary (2013 and 2014)

PUBLICATION STATISTICS

Total Publication:	213 (in peer reviewed journals)
Publication during 2012-17:	58 (in peer reviewed journals)
Cumulative Impact Factor (2012-17)	90.593
Total citation	2309 (on 24.06.2017)
Citation of the papers published during 2012-17	349
h-index	21

Conference/Symposia	Total: 268
Since 2012	International: 43 (invited 13), National: 40 (invited 13)

SELECTED PUBLICATIONS (since 2012)

11. Nabanita Naskar, Susanta Lahiri, Punarbasu Chaudhuri, Alok Srivastava, Measurement of Naturally Occurring Radioactive Material, ^{238}U and ^{232}Th : Anomalies in photo-peak selection J. Radioanal. Nucl. Chem. 310 (2016) 1381-1396.
10. Santu Maity, Susanta Lahiri and Jhuma Ganguly, Dynamic Chitosan-Based Self-Healing Hydrogels with Tunable Morphology and Its application in Separation Science RSC Adv. 6 (2016) 81060-81068
9. Susanta Lahiri, Moumita Maiti, Kaushik Gangopadhyay, Tracing ancient silk route by nuclear- analytical technique, J. Radioanal. Nucl. Chem 307 (2016) 225-228.
8. Santu Maity, Arpita Datta, Susanta Lahiri and Jhuma Ganguly, Selective Separation of ^{152}Eu from a Mixture of ^{152}Eu and ^{137}Cs Using Chitosan Based Hydrogel, RSC Adv. 5 (2015) 89338-89345.
7. Moumita Maiti, Kaustab Ghosh, T.M. Mendonça, Thierry Stora, **Susanta Lahiri**, Comparison on the production of radionuclides in 1.4 GeV proton irradiated LBE targets of different thickness, J. Radioanal. Nucl. Chem. 302 (2014) 1003-1011.
6. L. Gastaldo, K. Blaum, A. Doerr, C.E. Duellmann, K. Eberhardt, S. Eliseev, C. Enss, A. Faessler, A. Fleischmann, S. Kempf, M. Krivoruchenko, **S. Lahiri**, M.

- Maiti, Yu. N. Novikov, P.C.-O Rantizsch, F. Simkovic, Z. Szucs, M. Wegner, The electron capture ^{163}Ho experiment ECHO, *J. Low Temp. Phys.*, 176 (2014) 876-884.
5. J. Khuyagbaatar, A. Yakushev, Ch. E. Düllmann, D. Ackermann, L.-L. Andersson, M. Asai, M. Block, R. A. Boll, H. Brand, D. M. Cox, M. Dasgupta, X. Derkx, A. Di Nitto, K. Eberhardt, J. Even, M. Evers, C. Fahlander, U. Forsberg, J. M. Gates, N. Gharibyan, P. Golubev, K. E. Gregorich, J. H. Hamilton, W. Hartmann, R.-D. Herzberg, F. P. Heßberger, D. J. Hinde, J. Hoffmann, R. Hollinger, A. Hübner, E. Jäger, B. Kindler, J. V. Kratz, J. Krier, N. Kurz, M. Laatiaoui, **S. Lahiri**, R. Lang, B. Lommel, M. Maiti, K. Miernik, S. Minami, A. Mistry, C. Mokry, H. Nitsche, J. P. Omtvedt, G. K. Pang, P. Papadakis, D. Renisch, J. Roberto, D. Rudolph, J. Runke, K. P. Rykaczewski, L. G. Sarmiento, M. Schädel, B. Schausten, A. Semchenkov, D. A. Shaughnessy, P. Steinegger, J. Steiner, E. E. Tereshatov, P. Thörle-Pospiech, K. Tinschert, T. Torres De Heidenreich, N. Trautmann, A. Türler, J. Uusitalo, D. E. Ward, M. Wegrzecki, N. Wiehl, S. M. Van Cleve, V. Yakusheva, $^{48}\text{Ca} + ^{249}\text{Bk}$ Fusion Reaction Leading to Element Z = 117: Long-Lived α -Decaying ^{270}Db and Discovery of ^{266}Lr , *Phys. Rev. Lett.* 112 (2014) 172501-1 – 172501-5.
 4. Moumita Maiti, Santosh R. Tiwari, Nilesh B. Dubey, Hemlata Bagla, **Susanta Lahiri**, An improved method for determination of ^7Be in mosses, *J. Radioanal. Nucl. Chem.* 295 (2013) 1443-1446.
 3. Moumita Maiti, Ajoy Mandal, **Susanta Lahiri**, An improved non-destructive method of potassium determination, *Appl. Radiat. Isotopes* 71 (2013) 37-40.
 2. Ajoy Mandal, **Susanta Lahiri**, Production and separation of no-carrier-added ^{73}As and ^{75}Se from ^7Li irradiated germanium oxide target, *Radiochimica Acta* 100 (2012) 865-870.
 1. U. Forsberg, P. Golubev, L.G. Sarmiento, J. Jeppsson, D. Rudolph, L.-L. Andersson, D. Ackermann, M. Asaif, M. Block, K. Eberhardt, J. Even, Ch.E. Düllmann, J. Dvorak, J.M. Gates, K.E. Gregorich, R.-D. Herzberg, F.P. Heßberger, E. Jäger, J. Khuyagbaatar, I. Kojouharov, J.V. Kratz, J. Krier, N. Kurz, **S. Lahiri**, B. Lommel, M. Maiti, E. Merchán, J.P. Omtvedt, E. Parr, J. Runke, H. Schaffner, M. Schädel, A. Yakushev, First experiment at TASCA towards X-ray fingerprinting of element 115 decay chains, *Acta Physica Polonica B*, 43 (2012) 305-311.

TEACHING/GUIDANCE Degree Awarded (after 01.01.2012) **4/ On Board 03**
Total 13
 Teaching Post M. Sc, SINP, (Biophysical Sciences)

AREAS OF RESEARCH (2012-2016)

1. Nuclear and Radiochemistry
 - a. Physics and chemistry of accelerator produced neutron deficient radionuclides
 - b. Radiotracer technique
 - c. Physics and chemistry of converter targets
 - d. Superheavy elements, Accelerator Mass Spectrometry, etc.
2. Green Chemistry 3. Trace Analysis and Bio-monitoring

ESSENTIAL STRENGTH OF RESEARCH/DEVELOPMENT OUTPUT:

Throughout my 20 years career in SINP, I carried out most of my works in India in the field of Nuclear Chemistry using medium energy accelerators at VECC and BARC-TIFR Pelletron. However, I also collaborated with well known international institutions like CERN-ISOLDE, GSI, Germany (SHE collaboration with TASCA group); Heidelberg University, Germany; Institute of Modern Physics, China; TU Munich, Germany; ATOMKI, Hungary; Agricultural University, Debrecen, Hungary; TU Delft, Netherlands; ETH, Switzerland; St. Petersburg University, Russia.

Our work is associated with many “first.” In the early career, we started cyclotron production of no-carrier-added (NCA) radionuclides by alpha particle activation. We used thicker targets so that simultaneously many nuclear reaction channels open as the α -particles traverses through the target. This allowed us to produce a number of NCA radionuclides of different elements in single target matrix and afterwards we separated each NCA radionuclides in very pure state. We made for the first time exhaustive and systematic studies on heavy ion (like ^7Li , ^{12}C , ^{16}O , etc.) induced reactions to produce neutron deficient radionuclides. This investigation on both physics and chemistry of heavy ion induced reactions was well recognized internationally, as it gave the scientific community easy access of neutron deficient short-lived radionuclides. In fact our work on heavy ion activation is pioneering all over the globe and one of the reason for my Hevesy Medal Award. The most notable works in this field includes production of clinically important ^{199}Tl , $^{207-211}\text{At}$ and $^{93,94,95,96}\text{Tc}$ radionuclides.

The idea of “tracer packet” conceived and coined by us, is resurrection in the field of radiotracer technique. Since the discovery of radiotracer technique by George De Hevesy in 1923 only single tracer was used to investigate chemical and physical pathways. In 1991 Ambe et al. in RIKEN, introduced multitracer technique. In the year 20001, we introduced “tracer packet technique”, wherein multiple projectiles were used for production of radioisotopes of few closely associated elements simultaneously, and use of all these isotopes together helped to understand multielemental dependence of natural systems.

We developed methods of separation of minuscule amount of supernova produced radionuclides ^{53}Mn , ^{146}Sm and ^{182}Hf from the billion times abundant interfering stable isobars ^{53}Cr , ^{146}Nd and ^{182}W respectively. These separation schemes would bring new dimension to cosmochemistry and a step forward to solve astronomical puzzle.

For the first time we made a fine blend of “radiotracer technique” and “Green Chemistry” and introduced “Radio-Green Chemistry”. We reported first “radioactive gold nanoparticles” synthesized by simple addition of $\text{H}^{198}\text{AuCl}_4$ in polyethylene glycol (PEG). We showed that the introduction of minuscule amount of in situ radioactivity is useful for synthesis of gold palladium bimetallic nanoparticles. As a part of the green chemistry approach we used ionic liquids, bio-reagents, biopolymers and biocompatible polymers in radiochemical separation. One of his techniques earned international patent describing isolation of $^{199-201}\text{Tl}$ from the bulk lead target.

In the post Fukushima era, we realized compelling need for alternative source of radionuclide production. With the advent of high-energy physics, multi megawatt proton to neutron converter targets like liquid mercury or lead-bismuth eutectic (LBE) are planned worldwide, to build up the next generation high power radioactive ion beam (RIB) facility. We

proposed that these high power multi megawatt converter targets could be enormous source for radioisotope production if proper attention is paid by the radiochemists. For the first time, we made complete inventory of radionuclides of 1.4 GeV proton induced thick LBE targets. The results have impact in various interdisciplinary fields, such as understanding fundamental nuclear reactions in the high-energy domain, risk assessment for health safety, and as a source of clinical radionuclides.

On May 1, 2014, Physical Review Letters confirmed the existence of a new super-heavy element 117. In 2007, we joined the TASCAs group, GSI, Germany, contributed significantly and are the proud partners of E-114 and E-117 experiments. The TASCAs group also discovered two new isotopes ^{266}Lr and ^{277}Hs .

The ^{163}Ho radionuclide has half-life of 4570 years, has no alpha, beta or gamma rays but decays only by electron capture; therefore made this radionuclide unique for neutrino mass measurement. Our team for the first time proposed indirect way of production of ^{163}Ho via $^{163}\text{Dy}(\alpha, xn)^{163}\text{Er}(\epsilon)^{163}\text{Ho}$ or via $^{159}\text{Tb}(^7\text{Li}, 3n)^{163}\text{Er}(\epsilon)^{163}\text{Ho}$ reaction. This proposal has paramount importance in the relevant field like determination of exact mass of neutrino, and as a result a new international collaboration called ECHO collaboration (Electron Capture of Holmium neutrino) was formed. I am one of the founder members of this international collaboration.

FUTURE RESEARCH OR DEVELOPMENT PLAN

In future we would like to link between the research on fundamental sciences and its application towards the benefit of the society. We propose **REd TULIP**(Research and Education on Trace, Ultratrace Exposure and Isotope Production) as an umbrella project, an unique combination of Science for Society and Fundamental Research.

The vision of Nuclear and Radiochemistry Laboratory of CSD is to explore fundamental aspects of production of isotopes in different energy scale, from sub eV to GeV, development of their separation method and understanding the fundamental principle of working with few atoms. The science of radiotracer production is interdisciplinary combining physics, chemistry and biology. We would like to fully exploit the capability of upcoming medical cyclotron in Kolkata and the existing accelerators of VECC and TIFR to propose new radiotracer-bio-conjugate ligands, experimentally assess yield and cross sections of heavy ion induced reactions, especially on the neutron deficient sides of the radionuclidic chart.

Apart from using different existing accelerators, we will also pay our attention to the science and application of liquid lead bismuth eutectic (LBE) target, which is first predicted by us as possible enormous source of useful radionuclides, which became specially relevant after 2011 Fukushima Daichi accident, when public in general became hostile for the installation of new reactors world-wide and at the same time many of the old reactors had crossed the working time span and facing immediate shutdown. In Indian context, liquid lead has been proposed as target at the proposed ANURIB facility. LBE is also proposed in ADS systems in India. We would like to develop a virtual bank of different exotic radionuclides including their isolation and separation process from LBE target and entering in the new era of radioanalytical chemistry.

We would also like to work on the anthropogenic pollution and natural radioactivity assessment in Teesta and Hooghly river basin. Rivers are the arterial system

of Indian civilization that flushes out wastes to the ocean sinks. However, keeping in mind that rivers also provide for food and drinking water for most of the people in the country, cleaning is of utmost importance. Consequently, a lot of attention and resources has been mobilized towards Ganga, Brahmaputra and other big rivers mainly focusing on their water flow, flood and dams. We would like to shed light on some other aspects on two rivers, Teesta and its tributaries – the lifeline of Sikkim and North Bengal and on the mouth of the river Hooghly, especially on Sundarban area. It is worth noting that heightened interests to tame and exploit a river through dams, canals and hydel-power projects may increasingly expose population even beyond river basin to heavy metals and other contaminants directly or through bioaccumulation and bio-magnification. To assess the impact of upstream human activities and numerous stagnating dams on the tributary on course of river Teesta, trace analysis would be carried primarily on the river water and sediments as well as flora and fauna sample from the river basin. The other important aspect is to assess baseline radioactivity level in the sediments, water and soil samples surrounding Teesta and Hooghly river. Both Sundarban and Teesta could be affected by any unwanted nuclear incidents. Without baseline data it would not be possible to establish any increase in the level of radioactivity after such incidents. The radiotracer study will also be extended on the paleo-climate studies of Hooghly river basin as well as to unravel various archeological myths in this region to unravel our rich heritage.



Munna Sarkar

DOB:-27th September 1960

Professor-G

Chemical Sciences Division

Saha Institute of Nuclear Physics.

Educational background:

Passed B.Sc. and M.Sc from Calcutta University in Physics and completed Ph.D. in Physics (1994) from Saha Institute of Nuclear Physics, (Calcutta University). The thesis title was "Spectroscopic studies of some biologically important molecules"

Academic Profile:

► **March 1993 - August 1993:-** Post Doctoral Fellow in the group of Prof Astrid Gräslund (Secretary, Nobel Committee in Chemistry) at the Department of Medical Biochemistry and Biophysics in Umeå University, Umeå, Sweden.

► **August 1993 - June 1994 and from June 1995 till March 1998** continued working with her at the Department of Biophysics, Arrhenius Laboratories, Stockholm University Sweden.

► **December 1994 - June 1995:-** Visiting Fellow at the Biophysics Division, Saha Institute of Nuclear Physics, Calcutta, India.

► **1st April 1998 - 31st January 2000:-** Lecturer 'C', Saha Institute of Nuclear Physics.

► **1st February 2000 – 31st January 2004:-** Reader 'D', Saha Institute of Nuclear Physics.

► **1st February 2004 - 31st January 2007:-** Associate Professor 'E' Saha Institute of Nuclear Physics.

► **1st February 2007- 30th June 2012:-** Professor 'F' Saha Institute of Nuclear Physics.

► **1st July 2012 – Present:-** Professor 'G' Saha Institute of Nuclear Physics

Special Awards, honors or distinctions:

1) National Scholarship/Certificate of Merit for Secondary examination (1976) from Ministry of Education Govt. of West Bengal, India. 2) Prof. S. R. Palit Memorial award of The Indian Chemical Society for paper presentation December 1988. 3).Silver jubilee award of the Indian Society for Photobiology for poster presentation Feb 1989. 4. Awarded full fellowship by **ICTP Italy** to participate in the "**College on Methods and Experimental Techniques in Biophysics.**" (28th September to 23rd October 1992) held at the *International Centre for Theoretical Physics (ICTP). Trieste, Italy.*

Reviewer of the following journals:

1] Journal of Medicinal Chemistry (American Chemical Society), 2] Journal of Physical Chemistry: B (American Chemical Society), 3] Inorganic Chemistry Communication (Elsevier), 4] BBA: Biomembranes (Elsevier), 5] Langmuir (American Chemical Society), 6] Inorganica Chimica Acta (Elsevier), 7] Spectroscopy Letters, 8] International Journal of Biological

Macromolecules (Elsevier), **9**] *Frontiers in Biology*, **10**] *Journal of Photochemistry and Photobiology A: Chemistry* (Elsevier).

Reviewer of International/National Grant Proposals.:

- 1] Reviewer of grant proposals submitted to
NATIONAL SCIENCE CENTRE, ul. Królewska 57
30-081 Kraków, Poland <http://www.ncn.gov.pl/?language=en>
- 2] Reviewer of grant proposals submitted to West Bengal Department of Biotechnology

Management / Organizing Experience:

Served/serving the following committees of SINP between 2012-present.

- a) Medical Advisory Committee (**member**)
- b) Foreign Purchase Committee (**ex-member**)
- c) Inspire Faculty Recruitment Committee (**member**)
- d) Safety committee (**ex-member**)

Supervisor of Ph.D. work at SINP (Ph.D. degree awarded/ongoing during 2012-2016):

- 1) "NSAIDs induced membrane fusion." -Sutapa Mondal **Ph.D. degree awarded, November 2012, Jadavpur University, Kolkata.**
- 2) "Metal complexes of NSAIDs and their bio application. -Sreeja Chakraborty **Ph.D. degree awarded, December, 2014, Jadavpur University, Kolkata.**
- 3) "Effect of different physico-chemical properties of the drugs and the membranes on Non Steroidal Anti-Inflammatory Drugs induced membrane fusion." Anupa Majumdar **Ph.D. degree awarded, June 2016, Jadavpur University, Kolkata.**
- 4) "Identification of cellular signalling network which induces cancer cell death in response to certain drugs and natural products." Neha Rai (joint supervisor with Prof. Sanghamitra Raha C&MB Division) **Ph.D. degree awarded, November 2016, Calcutta University, Kolkata.**
- 5) "Molecular basis of alternate functions of NSAIDs" Sathi Goswami (**ongoing**)

Teaching experience (2012- 2016):

Post M.Sc. (Biophysical Science) course.

- a) Biomembranes (basic course)
- b) Drug discovery: a modern day approach (advanced course)
- c) Application of Fourier Transform Infrared and Circular Dichroism Spectroscopy in studying biomolecular structure and interactions (basic course).

Number of summer project students trained at SINP (2012- 2016). Five

Present Research (2012-2016):

New functions for old drugs: Non Steroidal Anti-Inflammatory Drugs (NSAIDs).

NSAID group of drugs are the most common drugs used to combat pain and inflammation. Besides these principal functions, they also show several other functions viz. chemoprevention and chemosuppression against different cancers, protection against neurodegenerative diseases, UV photosensitizer and UV photoprotector. The mechanism behind these diverse functions of NSAIDs is poorly understood. The aim of our group is to elucidate the molecular mechanism behind the different functions of NSAIDs such that the old drugs can be used more effectively for their alternate functions and can also be used as templates for future drug designing. The

molecular basis of these functions is probed using both biophysical and biochemical techniques. The main areas that have already been studied or are being studied since 2012 include.

I] Membrane fusion: A new function of NSAIDs

Membrane fusion, an integral event in several biological processes, is characterized by several intermediate steps guided by specific energy barriers. Hence, it requires the aid of fusogens to overcome the energy barriers to complete the fusion process. Common fusogens like proteins/peptides have the ability to overcome these barriers by their conformational reorganization, an advantage not shared by small drug molecules. Hence, drug induced fusion is a rare event. A few examples of drug induced membrane fusion that exists in literature, are shown to occur at a very high physiologically irrelevant concentration. *We have shown that all NSAIDs belonging to the oxicam chemical group viz. piroxicam, meloxicam lornoxicam and isoxicam and tenoxicam can cause membrane fusion at physiologically relevant concentration of the drugs and without the help of any other fusogenic agent.* To use drugs to induce and control membrane fusion in various biochemical processes requires the understanding of how different parameters modulate fusion. Effect of different physico-chemical parameters of both the participating drugs and the lipid bilayer of the membranes is being deciphered. [a) Anupa Majumdar, Debjyoti Kundu, and Munna Sarkar* **Journal of Physical Chemistry B. 119 (2015) 9627–9639.** b) Anupa Majumdar and Munna Sarkar* **Journal of Physical Chemistry B. 120 (2016) 4791–4802**].

II] Designing a new class of membrane anchors.

In an effort to increase the efficacy of membrane fusion of the oxicam NSAIDs, we have synthesized copper complexes of two oxicam NSAIDs viz. copper-piroxicam and copper meloxicam. Both the complexes show enhanced fusion efficacy over the free drugs. We have shown that their enhanced fusion efficacy is because of their ability to act as **membrane anchors** that can bridge apposing vesicles which help in initiating the first step of the fusion process. The existing designed membrane anchors present in literature are all based on two interacting partners incorporated in two sets of membranes. Interaction between the partners results in forming the bridge that initiates the first step of fusion. *The preformed copper complexes of NSAIDs have an edge over existing class of membranes anchors designed from interacting molecular partners. Unlike previously designed membrane anchors, for our designed anchors, both molecular recognition between molecular partners and the strength of interaction between them, do not play any role in membrane fusion.* [Anupa Majumdar, Sreeja Chakraborty, and Munna Sarkar* **Journal of Physical Chemistry B. 118 (2014) 13785–13799**]

III] DNA binding ability of the copper complexes of NSAID

NSAIDs form the most common class of anti-inflammatory and analgesic agents. They also show anticancer properties for which they exert their effects by interacting at the protein but not at the genomic level. This is because most NSAIDs are anions at physiological pH, which prohibit their approach to the polyanionic DNA backbone. Complexing NSAIDs with bioactive metal like copper obliterates this disadvantage. Copper complexes of piroxicam, meloxicam, lornoxicam and isoxicam have been synthesized and their ability to bind to the DNA backbone has been demonstrated. This binding is highly sequence selective. [a) Sreeja Chakraborty,¹ Esha Sehanobish² and Munna Sarkar* **Journal of Biological Inorganic Chemistry 17(2012) 475-487.** b) Sreeja Chakraborty, Madhuparna Bose, Munna Sarkar*. **Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy 122 (2014) 690–697.** c) Sathi Goswami, Suhita Ray¹, Munna Sarkar* **International Journal of Biological Macromolecules 93 (2016) 47-56**].

IV] DNA binding ability of the copper- NSAID complexes allows them to exert their effect at the epigenomic/genomic level (collaboration with Prof. Chandrima Das, SINP)

Complexing the NSAIDs with bioactive metals allow them to bind to the DNA, thereby, opening the possibility of genome level interaction. To test this hypothesis, we have done a comparative study on the interaction of a common NSAID, Piroxicam and its copper complex [Cu(II)-Px] with core histone and chromatin which resulted in structural alterations as monitored by different spectroscopic techniques and finally imaged by scanning electron microscopy. Such structural alterations can have different biological manifestations, but we have specifically focused on the changes at the epigenomic and genomic level to test the above mentioned hypothesis. The complex, [Cu(II)-Px], showed alteration of key epigenetic signatures implicated in transcription in the global context, although no significant changes were caused by Px. Subsequently, we have correlated such alterations caused by Cu(II)-Px with the changes in global gene expression by microarray analysis and validated the candidate gene expression alterations by qRT-PCR. Interestingly, cell viability was tested with MTT assay which indicated no significant damage in presence of both Px and [Cu(II)-Px]. Our study provided the first proof of concept that the copper complex of a traditional NSAID can exert its effect at the epigenomic and genomic level.

V] Piroxicam, a traditional non-steroidal anti-inflammatory drug (NSAID) causes apoptosis by ROS mediated Akt activation (Collaborator: Prof. Sanghamitra Raha, SINP)

Piroxicam (Px) belongs to the oxicom group of the non-steroidal anti-inflammatory drugs (NSAIDs) and have been shown to exert chemopreventive and chemotherapeutic effects in animal models and cultured animal cells. However, little is known about the mode of action of Px and its cellular targets. Our studies with human breast cancer cells MCF-7 showed that Px induced reactive oxygen species (ROS) generation along with apoptotic cell death. ROS release led to Akt activation. From our results, it became evident that ROS mediated apoptosis induction was due to Akt activation (hyper phosphorylation). Silencing the expression of Akt using siRNA and a specific Akt inhibitor, triciribine further confirmed the findings. However, Px failed to cause ROS generation, cell death or Akt phosphorylation in another human breast cancer cells MDA-MB-231 which is estrogen receptor negative and more aggressive compared to MCF-7 cells. This suggests that Px has cell type specific effects. Thus we showed for the first time that Px can induce apoptosis by ROS mediated Akt hyperphosphorylation. [*Neha Rai, Munna Sarkar* and Sanghamitra Raha** **Pharmacological Reports** 67(2015)1215-1223]

VI] Counterion effects on nano-confined metal–drug–DNA complexes (Collaborator: Prof. Alokmay Datta, SINP)

We have explored morphology of DNA molecules bound with Cu complexes of piroxicam (a non-steroidal anti-inflammatory drug) molecules under one-dimensional confinement of thin films and have studied the effect of counterions present in a buffer. X-ray reflectivity at and away from the Cu K absorption edge and atomic force microscopy studies reveal that confinement segregates the drug molecules preferentially in a top layer of the DNA film, and counterions enhance this segregation. [*Nupur Biswas, Sreeja Chakraborty, Alokmay Datta*, Munna Sarkar, Mrinmay K. Mukhopadhyay, Mrinal K. Bera and Hideki Seto.* **Beilstein Journal of Nanotechnology**, 7 (2016) 62-67]

VII] Detection of positional mismatch in oligonucleotides by electrochemical method (Collaborator: Prof. Amitabha De, SINP)

Detection of single base mismatch in DNA has been achieved by various techniques. However, the detection of position of that mismatch in the DNA duplex sequence has not been adequately addressed. In the present work, sensing of positional change of DNA base mismatch is achieved, with enhanced detection limit, using methylene blue as a redox indicator in electrochemical differential pulse voltammetric method (DPV). Interfacially synthesized Gold Polyaniline nanocomposites (Au-PAni) is coated on Pt electrode and attached with thiol modified single

stranded DNA to construct the sensor electrode. Position sensitive detection of a single base mismatch in oligomeric duplexes is achieved here, with a detection limit for concentration as low as 10^{-8} M for mixed oligomeric sequences and 10^{-6} M for dA-dT duplexes. In this case, the sensitivity of the electrode is $0.12\mu\text{A pM}^{-1}\text{cm}^{-2}$. Reusable sensor electrode coated with Au-PANI nanocomposites was employed without compromising the sensitivity of the system. This is the first step in developing a highly sensitive method for detecting the effect of varying position of single base mismatch in the DNA. [*Ankan Dutta Chowdhury, Nidhi Agnihotri, Amitabha De*, Munna Sarkar* **Sensors and Actuators B** 202 (2014) 917–923].

VIII] Lipid composition is an important determinant of antimicrobial activity of alpha-melanocyte stimulating hormone. (Collaborator: Prof. Kasturi Mukhopadhyay, JNU, New Delhi)

We have reported strong antimicrobial activity of cationic neuropeptide α -MSH against *Staphylococcus aureus*. Clinical *S. aureus* isolates non-susceptible to the peptide had higher amount of cationic phospholipid. To elucidate the molecular basis of lipid selectivity and antimicrobial activity of α -MSH, studies were carried out on SUVs having different combinations of neutral DMPC and anionic lipids DMPG to mimic mammalian and bacterial membrane. The peptide interacted with the DMPG containing vesicles only, as evident from the changes in Trp fluorescence. CD spectroscopy revealed that despite interaction, the peptide retained its native random coil structure. The perturbation of the vesicles caused by peptide interaction is strongly dependent on peptide concentration as seen both by DLS and Tb^{3+} /DPA based fluorescence leakage assay. Our data clearly demonstrate the preference of α -MSH to interact with anionic DMPG containing vesicles leading to significant permeabilization which is the molecular basis behind the selectivity of α -MSH for bacterial systems. [*Tahsina Shireen , Arnab Basub, Munna Sarkar, Kasturi Mukhopadhyay**. **Biophysical Chemistry** 196 (2015) 33–39].

Future areas of research:

- 1) Identifying the interaction of NSAIDs and their metal complexes at atomic details using theoretical approaches.
- 2) Application of the membrane fusogenic property of NSAIDs in cellular systems and its possible bio-applications.
- 3) Molecular basis of different extremophilic proteins: A theoretical approach.

List of Publications (2012-present): -

For citation details follow the url

<http://scholar.google.com/citations?hl=en&user=rly2wC4AAAAJ>

[**Journal Impact Factor as per ISI Web of Science Journal Citation Report (JCR) 2015, Citation as per ISI Web of Science]**

Average IF=3.189 (for 2012-present).

(*) **Principal/Corresponding author**

1. “Interaction of a Common Painkiller Piroxicam and Copper-piroxicam with Chromatin Causes Structural Alterations Accompanied by Modulation at the Epigenomic/Genomic level.”

Sathi Goswami, Sulagna Sanyal, Payal Chakraborty, Chandrima Das, Munna Sarkar**
Biochimica et Biophysica Acta (BBA) - General Subjects 1861 (2017) 2048-2059, [IF=5.083]
[Times cited=0] AU:- SINP=4, other=1

2. “Spectroscopic Studies on the Interaction of DNA with the Copper Complexes of NSAIDs Lornoxicam and Isoxicam.” *Sathi Goswami, Suhita Ray¹, Munna Sarkar** **International Journal of Biological Macromolecules 93 (2016) 47-56. [IF = 3.138] [Times cited=0] AU:- SINP=2 other=1 (summer project student)**

3. “Small Mismatches in Fatty Acyl Tail Lengths Can Effect Non Steroidal Anti-Inflammatory Drug Induced Membrane Fusion”. *Anupa Majumdar and Munna Sarkar** **Journal of Physical Chemistry B. 120 (2016) 4791–4802. [IF = 3.187] [Times cited=0] AU:- SINP=2**

4. “Counterion effects on nano-confined metal–drug–DNA complexes.” *Nupur Biswas, Sreeja Chakraborty, Alokmay Datta*, Munna Sarkar, Mrinmay K. Mukhopadhyay, Mrinal K. Bera and Hideki Seto.* **Beilstein Journal of Nanotechnology, 7 (2016) 62-67. [IF=2.778] [Times cited=0] AU:- SINP=6, other=1**

5. “Differential Effect of Oxicam Non-Steroidal Anti-Inflammatory Drugs on Membranes and Their Consequence on Membrane Fusion” *Anupa Majumdar, Debjyoti Kundu, and Munna Sarkar** **Journal of Physical Chemistry B. 119 (2015) 9627–9639. [IF = 3.187] [Times cited=1], AU:- SINP=2 other=1 (summer project student)**

6. “Piroxicam, a traditional non-steroidal anti-inflammatory drug (NSAID) causes apoptosis by ROS mediated Akt activation” *Neha Rai, Munna Sarkar* and Sanghamitra Raha** **Pharmacological Reports 67(2015)1215-1223. [IF= 2.251], [Times cited=0] AU:- SINP=3**

7. “Lipid composition is an important determinant of antimicrobial activity of alpha-melanocyte stimulating hormone” *Tahsina Shireen, Arnab Basu, Munna Sarkar, Kasturi Mukhopadhyay*.* **Biophysical Chemistry 196 (2015) 33–39. [IF = 2.363], [Times cited=4] AU:- SINP=2, other=2**

8. “Modulation of Non Steroidal Anti-Inflammatory Drug Induced Membrane Fusion by Copper Coordination of These Drugs: Anchoring Effect” *Anupa Majumdar, Sreeja Chakraborty, and Munna Sarkar** **Journal of Physical Chemistry B. 118 (2014) 13785–13799 [IF = 3.187], [Times cited=4] AU:- SINP=3**

9. “Detection of positional mismatch in oligonucleotides by electrochemical method” *Ankan Dutta Chowdhury, Nidhi Agnihotri, Amitabha De*, Munna Sarkar* **Sensors and Actuators B 202 (2014) 917–923. [IF=4.758], [Times cited=0] AU:- SINP=4**

10. “Spectroscopic studies of the binding of Cu(II) complexes of oxicamNSAIDs to alternating G-C and homopolymeric G-C sequences”. *Sreeja Chakraborty, Madhuparna Bose, Munna*

Sarkar*. **Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy** 122 (2014) 690–697 [IF=2.653], [Times cited=13] AU:- SINP=2 other=1 (summer project student)

11. “Binding of Cu (II) Complexes of Oxicam NSAIDs to Alternating A.T and Homopolymeric A.T Sequences: Differential Response to Variation in Backbone Structure” *Sreeja Chakraborty,¹ Esha Sehanobish² and Munna Sarkar** **Journal of Biological Inorganic Chemistry** 17(2012), 475-487. [IF=2.495] [Times cited=4], AU:- SINP=2 other=1 (summer project student)

Book Chapter

12. *Chakraborty H, Devi PG, Sarkar Munna *, Dasgupta D**. New Functions of Old Drugs: Aureolic Acid Group of Anti-Cancer Antibiotics and Non Steroidal Anti-Inflammatory Drugs. **Recent Advances in Medicinal Chemistry, Atta-ur-Rahman, Muhammad Iqbal Choudhary, George Perry (Editors), Bentham Science Publishers, Volume-1, 2014, pp 3-55. DOI: [10.2174/97816080579621140101](https://doi.org/10.2174/97816080579621140101) , eISBN: 978-1-60805-796-2, 2014; ISBN: 978-1-60805-797-9 ; ISSN: 2215-0722.**

Invited Talk (2012- 2016):

- 1] UGC Academic Staff College Jadavpur University, *Refresher Course on “Modern Chemical Sciences: Theories and Applications.” January 02-22, 2013.*
“Application of spectroscopy to identify new functions of old drugs”. *Munna Sarkar (invited talk)*
- 2] UGC Academic Staff College Jadavpur University, **Refresher Course on “Contemporary Teaching and Research in Chemistry” January 02-22, 2014**
“New functions for painkillers : membrane fusion”. *Munna Sarkar (invited talk).*
- 3] **National Symposium on Molecular Architecture, Dynamics and Assembly in Living Systems. Organizer: Indian Biophysical Society and Saha Institute of Nuclear Physics. Venue: Saha Institute of Nuclear Physics February 7-10, 2014**
“Anchoring Effect of Metal Complexes of fusogenic painkillers provides an edge over bare drugs in membrane fusion”. *Munna Sarkar* (invited talk)*
- 4] **102th Indian Science Congress: New Frontiers in Biology (Section) Venue: University of Mumbai, January 3-7, 2015.**
“New functions for old drugs: membrane fusion”. *Munna Sarkar (invited talk).*

MAITREYEE NANDY Professor G
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EDUCATION 2000: Ph.D. (Science) University of Calcutta
1990: Post M.Sc. (Radiological Physics),
Saha Institute of Nuclear Physics
1989: M.Sc. (Physics) University of Calcutta
(Session 1986-1988)
1986: B.Sc. (Physics Hons) University of Calcutta

ACADEMIC POSITION 2013 -: Professor G, Saha Institute of Nuclear Physics.
2007 – 2013: Professor F, Saha Institute of Nuclear Physics.
2004 – 2007: Associate Professor E, Saha Institute of Nuclear Physics.
2000 – 2004: Scientist D (Radiological Safety Officer), Saha Institute of Nuclear Physics.
1996 – 2000: Scientist SC, Saha Institute of Nuclear Physics.
1992 – 1996: Scientist SB in Saha Institute of Nuclear Physics.

EARLIER EMPLOYMENT DATA:

Physicist, Cancer Centre Welfare Home & Research Institute, February 1991-April 1992

AWARDS/ Visiting Scientist:

HONOURS a) Laboratori Nazionali di Frascati (INFN), Frascati, Italy: December 9, 2001 to March 8, 2002
b) Laboratori Nazionali di Frascati (INFN), Frascati, Italy: January 2, 2003 to February 15, 2003.
c) High Energy Accelerator Research Organisation, Tsukuba, Ibaraki, Japan; February 18, 2003 and April 20, 2003:
National Merit Scholarship, Madhyamik Pariksha, awarded by West Bengal Board of Secondary Education, Govt. of West Bengal.

PUBLICATION STATISTICS Journal: 61 (2012 – 2016: 18), Conference Proceedings: 67, Book Chapter: 1

SELECTED PUBLICATIONS Sabyasachi Paul, Maitreyee Nandy*, A. K. Mohanty, and Y. K. Gambhir. "Preequilibrium neutron emission in heavy ion reaction: Mean field effect and multiple emission" *Physical Review C* **94**, 034607 (2016)
(2012–2016) Maitreyee Nandy*, P K Sarkar, T Sanami, M Takada and T Shibata. "Neutron emission and dose distribution from natural carbon irradiated with a 12 MeV $\text{amu}^{-1} \text{ }^{12}\text{C}^{5+}$ ion beam" *Journal of Radiological Protection* **36** 456 – 473 (2016)

B.H.V. Pai, M. Nandy, A. Krishnamoorthy, P.K. Sarkar, Philip George. "Comparative study of Self-Compacting Concrete mixes containing Fly Ash and Rice Husk Ash." *American Journal of Engineering Research*, **03** (Issue-03) 150-154 (2014)

B.H.V. Pai, M. Nandy, A. Krishnamoorthy, P.K.Sarkar, C. PramukhGanapathy, Philip George. "Development of Self-Compacting Concrete with Various Mineral Admixtures." *American Journal of Civil Engineering*. **2** (3): 96-101 (2014). doi: 10.11648/j.ajce.20140203.16.

Sarkar, B.; Manikandan, A.; Nandy, M.; Gossman, M. S.; Sureka, C. S.; Ray, A.; Sujatha, N., A mathematical approach to beam matching, *British Journal of Radiology* **86** (1031), Article Number: 20130238 (Nov. 2013) **IF: 1.217**

Sunil C., T. Bandyopadhyay, M. Nandy, Vitisha Suman, S. Paul, V. Nanal, R.G. Pillay, P.K. Sarkar, Thick target neutron yield from 145 MeV $^{19}\text{F}+^{27}\text{Al}$ system, *Nuclear Instruments and Methods in Physics Research A* **721** 21-25 (2013) <http://dx.doi.org/10.1016/j.nima.2013.04.039> **IF: 1.207**

Sarkar, B.; Nandy, M.; Manikandan, A.; et al. "Estimation of Uncertainty in Dose Delivery Due to MLC Position Inaccuracies by Inverse Derivative Method During Volumetric Modulated Arc Therapy Delivery by Elekta Beam Modulator" *Medical Physics* **39** (6) 3715-3715 (2012) **IF: 2.83**

Manikandan, A.; Sarkar, B.; Nandy, M.; Sujatha, N, Mallik, S, Goswami, J, "Evaluation of Velocity Dependent Positional Error of Dynamic Multi Leaf Collimator During VMAT Delivery Using a Well Defined Mathematical Function" *Medical Physics* **39** (6) 3714-3714 (2012) **IF: 2.83**

Maitreyee Nandy, and Chirashree Lahiri "Radioactivity Generation in Pb and Pb-Bi alloys by Protons – A Comparative Study from MeV to GeV

Sunil, C.; Shanbhag, A. A.; Nandy, M. Tripathy, SP. Sahoo, GS. Joshi, DS. Kale, RM. Sarkar, PK. Sharma, DN "Neutron ambient dose equivalent from 5 MeV/u B-10, B-11, C-12, C-13 and O-16, O-18 projectiles incident on a thick Al target" *Radiation Measurements* **47** (10) 1035-1043 (2012) **IF: 1.177**

TEACHING/ Ph.D. awarded: 2 (in the period 2012 – 2016: 1), Thesis to be
GUIDANCE submitted: 1

Post-M. Sc. (Biophysics):	Radiation Physics & Safety
Post-M. Sc. (Expt. Physics):	Particle Detectors
Biophysics & Mol. Biology, CU:	Radioactivity
Biomedical Instrumentation, CU:	Radioisotopes and Nuclear Medicine

Ph.D. student (ongoing): **Sabyasachi Paul, BARC**, Homi Bhabha National Institute, Mumbai; Regn No: PHYS01201204009, date Jan 1, 2012 (ongoing) [Jointly with Prof. A. K. Mohanty, SINP]

Thesis title: "Study of Neutron Yield from heavy ion reactions using pre-equilibrium models"

Number of Summer project students (2012 – 2016): 29

Invited lecture (2012 – 2016) 9

1. Radiation Safety

Pre-Ph.D. course work, December 30, 2016, Department of Biophysics & Molecular Biology, University of Calcutta

2. Radiation Dosimetry for Medical and Industrial Application: Recent Developments

International Conference on Materials Science and Ionizing Radiation Safety and Awareness (ICMSIRSA-2016), January 28-30, 2016, Shivaji University, Kolhapur, Maharashtra.

3. Nuclear Reaction: Evolution towards Equilibration

Physics Department, National Institute of Technology Karnataka, Surathkal, Karnataka, March 28, 2016.

4. Neutrons: Journey from Source through Shield

20th National Symposium on Radiation Physics (NSRP-20), October 28-30, 2015, Mangalore University, Mangalagangothri, Karnataka

5. Nuclear reaction - Probing the nucleus before equilibration & 6. Heavy ion reaction at low energies and the HION model

Nuclear Physics Workshop on "Physics of Particles & Nuclei and related Instrumentation", January 27-31, 2015, Physics Department, Benaras Hindu University

7. Quality Assurance of Concrete for Radiological Safety

Manipal Institute of Technology, Manipal, Karnataka, March 7, 2014

8. Radiation Environment - Assessment, Measurement and its Impact

International conference RADENVIRON 2012, April 12-14, 2012 Babasaheb Bhimrao Ambedkar University, Lucknow, Uttar Pradesh, India,

9. Radiation in Space – Biological Effects

14 day Workshop in Fundamentals of Space Science and Technology, June 9, 2012, Kalpana Chawla Centre for Space and Nano-Sciences and Ramkrishna Mission Vivekananda Institute, Kolkata.

AREAS OF RESEARCH

Nuclear reaction studies

Neutron spectrometry, dosimetry; gamma dosimetry

Induced activity generation studies

Clinical dosimetry

Research / Development work/ Output

Radiation safety design for the facility was finalized. The Preliminary Safety Analysis Report (PSAR) for FRENA has been approved by Atomic energy Regulatory Board, Govt. of India. Consent to proceed with the construction for housing the facility has been obtained from the regulatory authority.

We have studied the influence of mean field and the entrance channel angular momentum, along with that of two-body interaction, on emission of nucleons in heavy ion reactions in the energy range of $\sim 10 - 30$ MeV/A. This study owes its significance to the fact that once population of different states is determined, emission probability governs the double differential neutron yield. Emission probabilities calculated using density distribution obtained from relativistic mean field (RMF) theory are lower, particularly at small emission energies, than those obtained from an empirical expression used earlier. The lower emission probability reduces the overprediction (obtained in our earlier model) of neutron emission at back angles. Influence of multiple preequilibrium (PEQ) emission has also been studied. At projectile energies $\sim 25 - 30$ MeV/A multiple PEQ emission can explain the measured spectrum well.

Neutron energy-angle distribution from low energy heavy ion reaction has important radiological consequence in similar accelerator facilities. Angular distribution of neutron dose / yield from Al target by 5 MeV/u B, C, O and 7.5 MeV/A ^{19}F projectiles have been measured. At 7.5 MeV projectile energy some PEQ contribution was observed.

Excitation function of long-lived radio nuclides generated in neutron induced reaction at 1-200 MeV on some commonly encountered targets in accelerator facilities have been analysed in the framework of direct, pre-equilibrium and compound nuclear reactions. It was observed that hybrid model incorporating multiple pre-equilibrium emission fairly well predict the total cross section in the projectile energy range of 1-20 MeV.

We have developed and studied Self-Compacting Concrete SCC using i) industrial by-products and ii) Rock samples of different geological compositions in Karnataka as coarse aggregates (CA) in preparation of SCC. Utilization of the treated industrial by-products will help to achieve an economical SCC mix, to improve the microstructure and the durability of concrete and provides solution to disposal problems and other environmental pollution issues. Use of locally collected rock samples will reduce the cost of concrete.

Elemental concentration in the rock samples collected from Karnataka was analysed for production of long-lived activity. Among the CA samples suitable for SCC composition, dolomite rock produces lowest activity for all the isotopes studied. If used in shielding, this will facilitate mitigating the prevailing radiological waste management problems during decommissioning of nuclear facilities.

A mathematical approach has been developed for quality assurance of the therapeutic beam profile from a medical linear accelerator. Precision and accuracy of dose delivery for a gantry-mounted (GS) detector system and couch-set (CS) detector system in the case of volumetric modulated arc therapy (VMAT) have been compared.

Future research/development plan

- i) Cross section and neutron spectrum analysis in low energy nuclear reaction
- ii) Dosimetry of Sr, Cs and other nanoparticles.



Padmaja P Mishra

Associate Professor-E
Chemical Sciences Division
Saha Institute of Nuclear Physics.

Educational background: Passed B.Sc. and M.Sc from Utkal University University in Chemistry and completed Ph.D. in Chemistry (2006) from IIT, Bombay.

Advisor: Prof. Anindya Datta, Professor of Chemistry

Title of the thesis: "Spectroscopic investigation of aggregation, Macromolecular interaction and Photophysics of biologically relevant fluorophores in organized assemblies."

Academic Profile:

Earlier employment data:

- 2011-Onwards : Saha Institute of Nuclear Physics, Associate professor
- 2007-2011: Post Doc, **The Pennsylvania State University**, University Park, Pennsylvania, USA
Mentor: Prof. Tae-Hee Lee, Assistant Professor of Chemistry and Biology.
- 2006-2007, Post Doc., **Lehigh University**, Bethlehem, Pennsylvania, USA
Mentor: Prof. Tianbo Liu, Assistant Professor of Chemistry.

Member of Professional Bodies:

- i. American Chemical Society, USA
- ii. Biophysical Society, USA
- iii. The International Society for Optics and photonics
- iv. Indian Biophysical Society
- v. Indian Chemical Society

Reviewer of the following journals:

- a) Journal of Physical Chemistry: B (American Chemical Society)
- b) Optics later
- c) Spectroscopy Letters
- d) BBA: Molecular cell Research (Elsevier)
- e) Journal of Applied Spectroscopy (Springer)

Management / Organizing Experience:

Served/serving the following committees of SINP between 2012-present.

Warden, Students Hostel, MSA 1
 Member of Workshop Committee
 Member of Disaster management and safety Committee
 Doctoral Committee for Research Fellow at SINP
 The seminar coordinator for Chemical sciences division
 Coordinator of Chemical sciences departmental meetings
 Member of Students' welfare committee

PhD students since 2012

Sl No	Name	Joined SINP for Post MSc	Joined My laboratory for PhD Work	Present Status
1	Subhas Bera	2010	2013 (Till 2013, He was at Prof. Soumen Basaks Lab for Phd, and joined my group in March 2013)	Thesis Submitted, Joined as Postdoc at TIFR, Hyderabad
2	Tapas Paul	2012	2013.	5000 (Pre-thesis) Presented, Thesis will be submitted before 31 st July, 2017
3	Samrat Basak	2015	2016.	Continuing

Important equipment and facility: List of new equipment and facilities has been introduced to the division or the Institute which include:

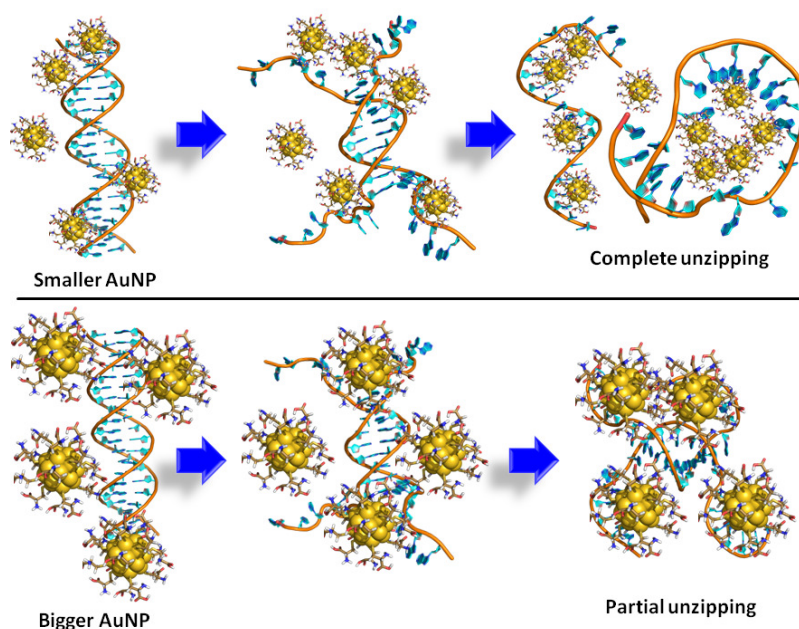
- (i) Two color, three color and four color Single molecule FRET imaging set up for real time monitoring of complex biological systems
- (ii) FRET-Anisotropy set up for real time monitoring of complex biological systems taking one molecule at a time
- (iii) Single Beam Optical tweezers for tracking and manipulation of small microscopic particles/ molecules etc
- (iv) FRET based Fluorescence correlation spectroscopy and fluorescence cross correlation spectroscopy at single molecule resolution.

(v) Research highlight (last 5 years and future plan):

i). Conformational changes and complete unzipping of dsDNA by surface modified Gold Nanoparticles (*The Journal of Physical chemistry B*, 2016, **Impact factor: 3.2**)

We have monitored the complete unzipping of DNA double helix by surface modified gold nanoparticles. It has been seen that nanoparticles of approximately 3-4 nm size with positive charge surface work collectively to carry out the entire process. We believe as the gold nanoparticles has positive charge, the DNA and nanoparticles were pulled together to form two single strands. The positively charged ligands on the nanoparticles attached to the DNA, and the hydrophobic ligands of the nanoparticles became tangled with each other, pulling the nanoparticles into clusters. At the same time, the nanoparticles pulled the DNA apart.

This work provides insight into the interaction of dsDNA with surface modified gold nanoparticles bearing very less surface charge density compared to a histone octamer. We have observed a collaborative effect of the nanoparticles resulting structural changes, compaction and strand separation depending on the size and hence charge on the AuNPs. Moreover, this opens up to explore the exact sequence of structural changes that the DNA experience and if it is sequence specific at all. Thus the results establish an alarming message to tune and balance the charges around the nanoparticles properly before using them for different therapeutic and other application. The interpretation of the results are mostly based on Single molecule FRET experiments, with other supporting techniques as used as well, namely: steady state and time resolved spectroscopy, circular dichroism spectroscopy, Viscosity measurements, Zeta Potential and imaging by Transmission Electron Microscope.

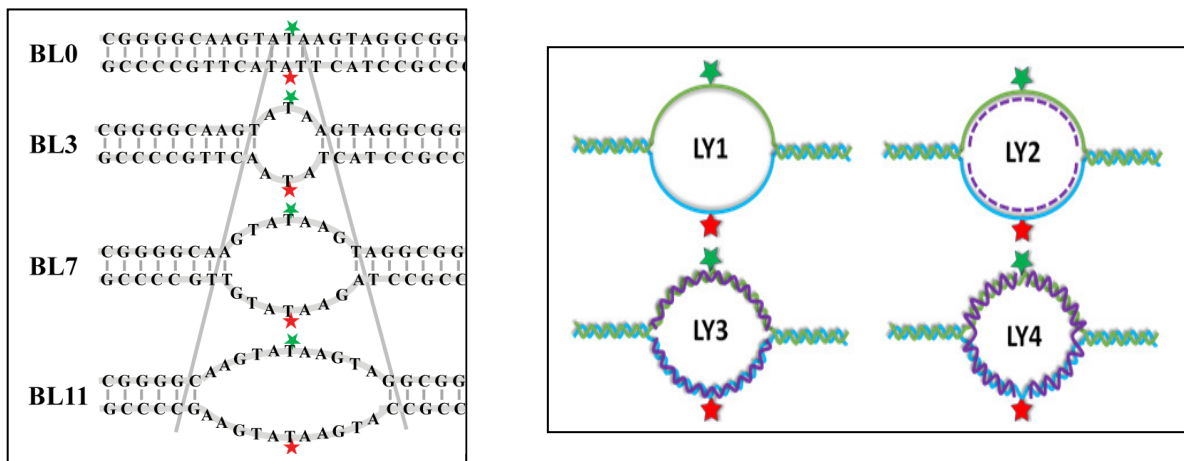


Scheme 1: Representation of the plausible mechanistic way of dsDNA unzipping in presence of surface modified AuNP. The upper panel represents the complete unzipping of the dsDNA after experienced a conformational change due to interaction with the 4 nm AuNPs. The lower panel represents the conformational changes and partial unzipping of dsDNA, when interacts with the bigger size (10 nm) AuNPs.

ii). **Bubble dynamics and DNA flexibility in presence of base pair mismatch**
(Manuscript Published in RSC Advances, Impact factor: 3.4 and Nanoscale, Impact factor: 7.8)

The genetic information preserved in chaotic universe through extraordinarily accurate duplication of DNA during cell division. Therefore, it is absolutely essential to make sure that the coded genetic information in DNA could always be retained properly. Though, most of the conformational changes in DNA are known to be driven by proteins and the binding have traditionally been discussed in terms of static structure; thermal denaturation also known to play an important role during this important process, as spontaneous bubble formation happens due to thermal fluctuations. Dynamics of the thermally induced DNA bubble formation shows spontaneously zipping- unzipping rate to follow multistate relaxation kinetics with a characteristic time scale of 50 μ s, (1) as the damage sites behave similar to that of ssDNA. Though increase in bubble size has been seen to induce an increase in the overall DNA length, it would also result in the increase in the equatorial bubble distances too. However, most of the research in this field have been concentrated on the overall DNA flexibility and bending of mismatch induced bubble DNA, and less has been explored on the dynamics of bubble portion, to counter to contradictory observations, if any. Mainly, if a change in the number of mismatch induces any change in the shape of the bubble area and in particular, the orientation of the two strands in the bubble region has not been scrutinized to a great extent.

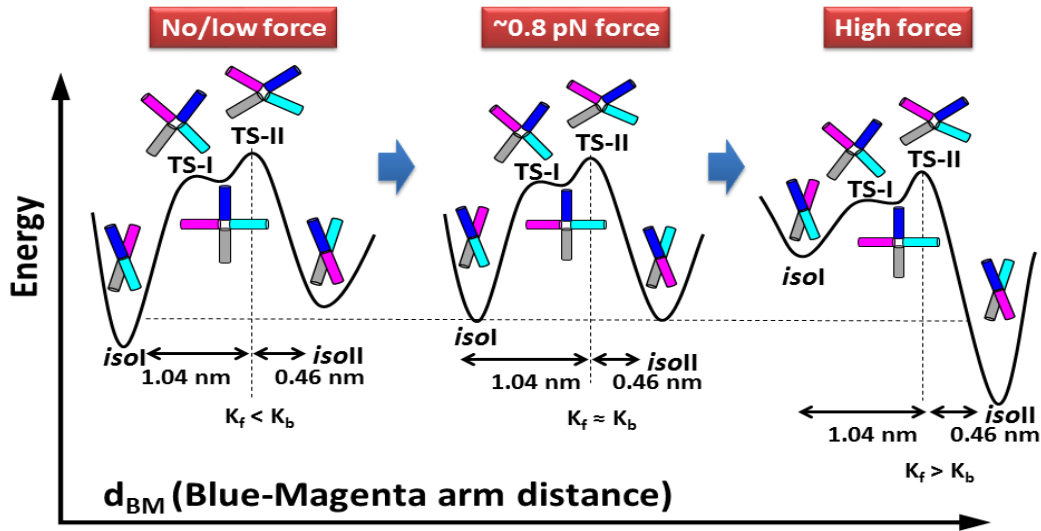
As a first step in addressing the above issues, we have investigated the nature of bubble using small DNA containing 23 nucleotides and having preferred nucleotide sequence nearly identical to that of the transcription initiation sequence. Our observations are based on the outcomes of experiments to trap the intermediate states by the use of ensemble and single molecule FRET techniques. Selective introduction of base pair mismatch for creation of melting bubble affects the local base stacking, along with the base pairing.



Scheme 2 The schematic representation of four sets of dsDNA having 23 nucleotides on each strand and labelled at the middle with Cy3 (green star) on one strand and Cy5 (red star) on the complementary strand, so that once annealed the FRET pair remains opposite to each other. Non Watson-Crick bp introduces bubble at the middle, whereas both of the ends are clamped by relatively strong Watson-Crick base pairing.

iii). Chaotic Dynamics During the Restricted Branch Migration of IHF Bound Holliday Junctions due to Applied Force: A smFRET study (Manuscript under revision)

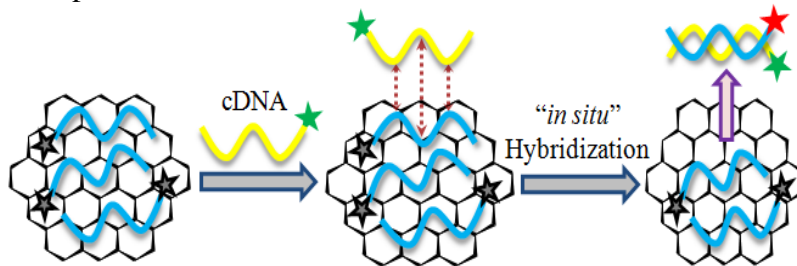
We have monitored the enhanced rigidity and reduced flexibility that a Holliday junction experiences upon binding to a DNA binding/Bending Protein, IHF. Though the transitions between alternative stacking conformers for four-way DNA junction as such has been investigated, stoichiometries of active molecular complexes and the internal conformations of this important structure, when bound to DNA binding protein is not clear. Using single molecule FRET technique, we have been able to detect the isomerization dynamics in presence of applied force. The introduction of nonlinear phase space analysis of the FRET signals quantitatively insight into the dynamics with increase in applied force. We have observed a restricted branch migration, once bound to IHF, and share the unstacked open structure with different rate-limiting steps. Furthermore, they have been observed to repeatedly sample distinct regions of the folding landscape over a long observation time. The associated folding landscape of the HJ is visualized in terms of rarely interconverting states embedded into the two isoforms, using nonlinear analysis. It is worth noting that although we have used Holliday junction as an example to explore quantitatively the concept of heterogeneity due to applied force, our conclusions are far reaching. Our study not only opens up new aspects of HJ-protein interactions, this concept is also expected to be applied to study protein-DNA interaction and effect of junction binding protein in recombination, irrespective of presence of applied force.



Scheme 3. Mapping of potential energy landscape of 4WHJ over different applied force. Y-axes represent the relative activation energy and the X-axes provides separation of blue-magenta arms. At no/low force, the *isoI* conformation is of lower energy hence with higher population compared to *isoII*. As the applied force increases, the energy landscape tilts towards *isoII* conformer and the potential energy of *isoII* become almost similar to that of *isoI* at ~ 0.8 pN force, resulting nearly equal population of both the conformers. However, for higher force, the opposite phenomena are observed.

iV). Single molecule FRET Studies of Hybridization mechanism during the noncovalent adsorption and desorption of DNA on Graphene Oxide. (Manuscript Published in the Journal of Physical chemistry B, Impact factor: 3.2)

The nature and strength of interaction between DNA and its components with synthetic molecules capable of DNA-binding has resulted in the development of several classes of designed scaffolds accounting to their unique physio-chemical properties. This particular work of our group provides insight into the interaction of DNA with low dimensional material 'Graphene Oxide' (GO) to give a detail hybridization mechanism during the adsorption and desorption of DNA on its surface. Our results depict the fundamental mechanism during the interaction and set the stage for formulating GOs as carriers of nucleic acids. The outcomes obtained emphasize the postulation of a parallel mechanism that can serve as basis for the further design and optimization of GO-based DNA sensor. The interpretation of the results is mostly based on ensemble and Single molecule FRET experiments.



Scheme 4. Representation of the proposed ds-DNA hybridization mechanistic pathway on the GO surface.

Future work:

- a) Transcriptional activation by protein-induced DNA bending: Mechanisms of protein–DNA recognition
- b) Single-molecule counting of cancer biomarker RNAs in human biofluids
- c) Improved understanding of the detailed Dynamics of superhelical DNA

List of Publications

Sl NO	Title	Name of Co Authors	Name of the Journal	Present Impact factor	Year of Publication	No Of Citations	No of Authors from SINP
1	Direct Observation of Breathing Dynamics at the Mismatch Induced DNA Bubble with nanometer accuracy: a smFRET Study	Tapas Paul, S. C. Bera, P P Mishra	Nanoscale	7.8	Mar, 2017	-	3
2	Direct observation of spatial configuration and structural stability of locked Y-shaped DNA structure	Tapas Paul, P P Mishra	Rsc Advances	3.3	11 th Oct 2016	1	2
3	Single molecule FRET Studies of Hybridization mechanism during the noncovalent adsorption and desorption of DNA on Graphene Oxide.	Tapas Paul, Subhas. C Bera, Nidhi Agnihotri, P P Mishra	Journal of Physical Chemistry B	3.2	12 th Oct 2016	1	4
4	Conformational Changes Followed by Complete Unzipping of DNA Double Helix by Charge-Tuned Gold Nanoparticles	Subhas C Bera; Kasturi Sanyal; D Senapati, P P Mishra	Journal of Physical Chemistry B	3.2	May, 2016	3	4
5	Conformational changes and unzipping of DNA by surface modified gold nanoparticle	Kasturi Sanyal; Subhas C Bera; Dulal Senapati; P P Mishra	Chem. Phys	1.75	Sep, 2011		4

MONTU K. HAZRA, Associate Professor E

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Email h.montu@saha.ac.in



EDUCATIONS

2008: Ph.D. in Science, Indian Institute of Technology Kanpur
2000: M.Sc. in Chemistry, University of Kalyani; 1st Class
1998: B.Sc. Chemistry Honours, The University of Burdwan; 1st Class

ACADEMIC POSITIONS

2012- Associate Professor E , Saha Institute of
.....: Nuclear Physics
2008- Post Doctoral Employee, University of
2011: California-San Diego
2008- Senior Project Associate, Indian Institute of Technology Kanpur
2008:
2007- Project Scientist, Indian Institute of Technology Kanpur
2008:
2002- Research Fellow, Indian Institute of Technology Kanpur
2007:

AWARDS/ HONOURS

- **Award for the Member of [American Chemical Society](#) (2015-18).**
- Reviewer of papers submitted in peer-reviewed International Journals (Journal of Chemical Sciences, Journal of Physical Chemistry, Physical Chemistry Chemical Physics, Chemical Physics Letter, etc).
- Jury Member, West Bengal, National Science Talent Search Examination (Vidyarthi Vigyan Manthan 2016-17).
- Invited to Chair a Session in the Discussion Meeting on Spectroscopy and Dynamics of Molecules and Clusters-2016 (SDMC-2016).
- Selected as one of the Resource Person in the Science Workshop on "Learning by Doing: Science Mysteries Demystified" 2014. Organized by Ramananda College, West Bengal, India.
- Board Member for the Scientific Creativity Test (Final Step) of Jagadish Bose National Science Talent Search (JBNSTS-2012) Examination.
- Qualified National Eligibility Test (NET) in Chemical Sciences in 2001.
- Qualified Graduate Aptitude Test in Engineering (GATE) in 2002 (**Percentile 99.5, All India Rank 13**).
- Junior Research Fellowship Award from Indian Institute of Technology Kanpur, India, 2002.
- Senior Research Fellowship Award of the Council of Scientific and Industrial Research (CSIR) India, 2004.
- Best poster award in National Symposium on Radiation and Photochemistry, 2005.

PUBLICATION STATISTICS

Journals: 23 (for 2012-2016: 6); *h*-index: 9

SELECTED PUBLICATION (2012-2016) as Corresponding Author (*)

- 1. Impact of OH radical-initiated H₂CO₃ Degradation in the Earth's Atmosphere via Proton-Coupled Electron Transfer Mechanism, S. Ghoshal and M. K. Hazra*, J. Phys. Chem. A 120, 562-575 (2016).**
 - The decomposition of isolated carbonic acid (H₂CO₃) molecule into CO₂ and H₂O (H₂CO₃ → CO₂ + H₂O) is prevented by a large activation barrier (>35 kcal/mol). Nevertheless, it is surprising that the detection of the H₂CO₃ molecule has not been possible yet and hunt for the free H₂CO₃ molecule has become challenging not only in the Earth's atmosphere but also on Mars. The present study shows that although the atmospheric concentration of the OH radical is substantially lower than the concentrations of the H₂O, formic acid (FA), Acetic acid (AA) in the Earth's atmosphere, but nevertheless, the OH radical-initiated H₂CO₃ degradation reaction has significant impact, especially, towards the loss of H₂CO₃ molecule in the Earth's atmosphere.
- 2. H₂CO₃ --> CO₂ + H₂O Decomposition in Presence of H₂O, HCOOH, CH₃COOH, H₂SO₄ and HO₂ Radical: Instability of the Gas-Phase H₂CO₃ Molecule in Troposphere and Lower Stratosphere, S. Ghoshal and M. K. Hazra*, RSC Adv. 5, 17623-17635 (2015).**
 - Gas-phase carbonic acid molecule (H₂CO₃) is an elusive species and its detection in the Earth's atmosphere as well as in outer space has become very challenging to a new generation scientists. In this work, we show that the gas-phase carbonic acid molecule in the Earth's atmosphere is an unstable species and it decomposes into its constituent CO₂ and H₂O in the presence of atmospheric water and carboxylic acids.
- 3. Autocatalytic Isomerizations of the Two Most Stable Conformers of Carbonic Acid in Vapor Phase: Double Hydrogen Transfer in Carbonic Acid Homodimers, S. Ghoshal and M. K. Hazra*, J. Phys. Chem. A 118, 4620-4630 (2014).**
 - The results of this study specifically and strongly suggest that double hydrogen transfer within the eight-membered cyclic doubly hydrogen-bonded (H-bonded) ring interface of the H₂CO₃ homodimer is ultimately the starting mechanism for the isomerization of the carbonic acid, especially, during the sublimation of the H₂CO₃ polymorphs at cold temperature (210-260K).
- 4. Hydrolysis of Glyoxal in Water-Restricted Environments: Formation of Organic Aerosol Precursors through Formic Acid Catalysis, M. K. Hazra*, J. S. Francisco* and A. Sinha*, J. Phys. Chem. A 118, 4095-4105 (2014).**
 - This article describes how glyoxal-diol and glyoxal-tetrol might be formed under atmospheric conditions associated with water-restricted environments. In addition, present work also strongly suggest that the formation of these precursors for secondary organic aerosol growth is not likely restricted solely to the bulk aqueous phase as is currently assumed.]

5. **New Mechanism for Autocatalytic Decomposition of H₂CO₃ in the Vapor Phase**, S. Ghoshal and **M. K. Hazra***, *J. Phys. Chem. A* 118, 2385-2392 (2014).
 - Carbonic acid (H₂CO₃), a small molecule of six atoms involving three elements in the periodic table, is right at the interface between organic and inorganic chemistry. At room temperature, this molecule is an unstable and elusive species as it decomposes rapidly into CO₂ and H₂O molecules. However, in the vast literature of carbonic acid, it was not known how carbonic acid decomposes into its constituents CO₂ and H₂O molecules. This article describes that the primary mechanism for the decomposition of carbonic acid is autocatalytic, especially at its source, where the vapor phase concentration of H₂CO₃ molecules reaches its highest levels.

6. **Gas Phase Hydrolysis of Formaldehyde To Form Methanediol: Impact of Formic Acid Catalysis**, **M. K. Hazra***, J. S. Francisco* and A. Sinha*, *J. Phys. Chem. A* 117, 11704-11710 (2013).
 - This article describes computational studies for a new mechanism for the diol formation catalyzed by formic acid. More generally, the results of this study have important mechanistic ramifications for how the gas phase hydrolysis of carbonyl compounds, which is the forbidden process in presence of single water molecule in our atmosphere, can be catalyzed by organic acids in the atmosphere.

TEACHING/GUIDANCE

Ph.D. Student: 1 (Ongoing), Summer Student: 1

Introduction to Quantum Mechanics (Chemical Biology and Biophysics)

Spectroscopy (Advance Course)

Research Methodology

National/International Conferences

Invited Talk: 2; Poster: 2; Organized: 1; Chairperson: 1

RESEARCH AND DEVELOPMENT

Current Project: Discovery of the New Reactions or New Mechanisms of Potential Atmospheric Importance for the Earth, Mars and Outer Space

In this project, both the energetics and kinetics of the new reactions or new mechanisms are explored as accurate as possible to find the potential impact of the reactions over existing or currently accepted reactions or mechanisms. At present, we use Quantum Chemical Calculations, Statistical Thermodynamics, Conventional Transition State Theory (CTST), Canonical/Micro-canonical Variational Transition [CVT, μ VT(E), E,J]- μ VT] State Theories, Hard-Sphere Collision Theory (HSCT) and Variable-Reaction-Coordinate-Variational Transition State Theory (VRC-VTST) to explore the potential impact of the reactions. Nevertheless, and in future, we are also looking forward for the experimental verifications of the proposed reactions in our laboratory.

Development:

Molecular Beam Chamber with Vacuum Pumping System for the detection of Laser

Induced Fluorescence in Supersonic Jet has been build successfully.

Future Research/Development

We are in the process of setting up a strong interdisciplinary research program in experimental physical chemistry and our research interests will span a broad range of areas covering the application of several spectroscopic techniques to investigate the gas phase molecules/complexes—which are important in atmospheric chemistry as well as in biological chemistry. Research projects in our laboratory will be directed toward investigating the gas phase spectroscopy and dynamics of the isolated molecules and their clusters. Both electronic and infrared spectroscopy in combination with laser induced fluorescence and time of flight mass spectrometric detections will be performed extensively to explore largely the structures, vibrations, photochemistry and photophysics of important isolated molecules, and in particular, their hydrogen-bonded (H-bonded) and van der Waals complexes. In the case of biologically related molecules, depending upon the size and nature of the molecules such as whether the molecules are non-volatile or thermo-labile, where cold gas-phase molecule preparation in supersonic jet environment does not work well, laser desorption method will also be coupled with mass spectrometric detections. In addition, quantum chemistry calculations will also be performed extensively to support our experimental results as well as for the preliminary investigations of systems/problems that we will address in our laboratory. At the present moment we decided to address two main future projects as mentioned below:

Project I: Infrared Spectroscopy, Photochemistry and Dynamics of Several Important Molecules and Their Hydrogen-Bonded Complexes Related to Atmospheric Chemistry

- This project is devoted to improve our understanding the atmospheric chemistry at the molecular level. In our atmosphere, the energy comes from the Sun mainly in the form of visible light and when this light reaches our earth through atmosphere, earth-surface becomes warm and radiate infrared radiation back into space in the form of heat. Therefore, infrared spectroscopy including both the fundamental and overtone transitions of the atmospheric constituents and their complexes in the laboratory, which are interconnected with atmospheric measurements, is highly important. In this research project, the State Resolved Photo-Dissociation Spectroscopy, commonly known as Vibrational Mediated Photodissociation (VMP) Spectroscopy will be performed extensively via the combinations of lights such as infrared, visible and ultraviolet. The VMP spectroscopy is known as a powerful and sensitive technique to record the infrared spectra over other various direct absorption techniques such as conventional FT-IR spectroscopy, laser photoacoustic spectroscopy or cavity ring down spectroscopy. It is worth noting here that higher overtone absorptions of atmospheric species containing O-H/N-H/C-H functional groups fall in the visible region of Sun-light and molecules containing O-H chromophores are

always under the attention of atmospheric chemistry because in presence of both UV and visible lights these molecules may lead to OH radicals, known as the primary sink for atmospheric pollutant. Furthermore, it has been also claimed that absorption of solar radiation by hydrogen-bonded (H-bonded) complexes, particularly those containing water, in the earth atmosphere is significant to climate change and H-bonded complexes can potentially influence climate through the absorption and scattering of solar radiation. Infrared spectroscopy can, in principle, provide a direct window to probe the H-bonded stretching coordinate of these complexes. To measure the infrared spectra of several important molecules and their H-bonded complexes related to atmospheric chemistry, we are in the process to develop the successful set up for the Vibrational Mediated Photodissociation (VMP) Spectroscopy.

Project II: Electronic and Infrared Spectroscopy of Small Units of Biologically Related Molecules and Hydrogen-Bonded Complexes Mimicking Nucleobase Pair Analogues

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This project is devoted to learn precisely about their intrinsic hydrogen-bonding/stacking/van der Waals interactions and dynamics via hydrogen-bonding interfaces. In this research project, various convenient species/systems will be designed and generated in the gas phase by either supersonic jet or laser desorption environments to get good testing grounds in resolving many of the complexities found in larger complex molecular network. Intramolecular N-H/O-H-stretching fundamental vibrational frequencies of intramolecular H-bonded molecules as well as inter-molecular H-bonded complexes will be measured by the use of sophisticated double and triple resonance techniques such as IR-UV (Infrared-Ultraviolet) and IR-UV-UV (Infrared-Ultraviolet-Ultraviolet).

Future Development:

Time of Flight Mass Spectrometer with Pulsed Electron Gun in the Ionization Chamber has been designed successfully to build it as soon as possible.



DULAL SENAPATI,

Associate Professor, E

DoB 17 December 1974

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EDUCATION

2004: Ph.D. Experimental Chemical Physics, Indian Institute of Science, Bangalore, India
Photodissociation Dynamics of Mixed Halogenated Alkyl and Aryl Halides (Advisor: P. K. Das)

1988: M.Sc. in Chemistry (Physical Chemistry special), Jadavpur University, Kolkata, India

1996 B. Sc. Chemistry Hons, Vidyasagar University, Midnapur, India

ACADEMIC POSITIONS/PROFESSIONAL RESEARCH EXPERIENCE

Saha Institute of Nuclear Physics, Calcutta, WB 700064-Associate Professor

2013-

SERS & SEHRS, Ultrafast Surface Dynamics, Electron Microscopy Based Nano-Materials Structural Evolution, Controlled Nano-Architecture, Solid State Renewable Energy
Jackson State University, Jackson, MS 39217-Research Associate

2008-2012

Real Time Nano-materials Evolution, Synthesis and Photophysics of Nanomaterials, Nanomedicine, Nano-materials-based Chemical & Biological Sensor (**Supervisor: P. C. Ray**)
Material Research Laboratory, UCSB, Santa Barbara, CA 93106-Visiting Scientist

2009

Magnetic Nano materials, Polymer-based Nano-Composite (**Collaborator: Craig J. Hawker**)
Georgia Institute of Technology, Atlanta, GA 30332-Postdoctoral Fellow

2005-2008

Single Molecule Raman and Fluorescence imaging, Dendrimer and DNA encapsulated Fluorescent Nano-clusture Synthesis, Ag-Nanoparticle-based Solid State Solar Cell, Femtosecond Electron Injection Dynamics (**Supervisor: Robert M. Dickson**)

Indian Institute of Science, Bangalore, India-Graduate Student

1998-2004

Gas Phase Photodissociation Dynamics, Laser Spectroscopy, Non-Linear Optics, Laser Ablation, Polymer Degradation, Photodynamic Therapy (**Supervisor: P. K. Das**)

Reviewer of papers submitted in peer-reviewed International Journals

ACS, Elsevier, RSC, Springer, Willey, etc.

PUBLICATION STATISTICS

Citations: 3452, h-index: 27, i10-index: 39

PUBLICATIONS after joining SINP

1. Characterization of Bimetallic Core-Shell Nanorings Synthesized via Ascorbic Acid Controlled Galvanic Displacement followed by Epitaxial Growth, T. Ghosh, B. Satpati*, D. Senapati, Journal of Materials Chemistry C **2014**, 2, 2439-2447.
2. Synergistically-Controlled Nano-Templated Growth of Tunable Gold Bud-to-Blossom Nanostructures: A Pragmatic Growth Mechanism, M. Bardhan, B. Satpati, T. Ghosh, D. Senapati*, J. Mater. Chem. C **2014**, 2, 3795-3804.
3. Effect of intertip coupling on the plasmonic behavior of individual multitipped gold nanoflower, Achyut Maity, Arpan Maiti, Pabitra Das, Dulal Senapati, Tapas Kumar Chini, ACS Photonics **2014**, 1, 1290-1297.
4. Charge Density Modulated Shape-Dependent Electrocatalytic Activity of Gold Nanoparticles for the Oxidation of Ascorbic Acid, Debranjana Mandal, Subrata Mondal, Dulal Senapati, Biswarup Satpati, Marthi V Sangaranarayanan, J. Phys. Chem. C **2015**, 119, 23103-23112.
5. A Supramolecular hydrogel for generation of a benign DNA-hydrogel, B. Dey, R. K. Mondal, S. Mukherjee, B. Satpati, N. Mukherjee, A. Mandal, D. Senapati, S. P. Sinha Babu, RSC Advances **2015**, 5, 105961-105968.
6. Conformational Changes Followed by Complete Unzipping of DNA Double Helix by Charge-Tuned Gold Nanoparticles, Subhas C. Bera, Kasturi Sanyal, Dulal Senapati, Padmaja P. Mishra, J. Phys. Chem. B **2016**, 120, 4213-4220.
7. Direct experimental observation of salt induced aspect ratio tunable PFPT silver-nanowire formation: SERS-based ppt level Hg²⁺ sensing from ground water, M. Bhattacharya, A. R. Mandal, S. Das Chakraborty, Arpan Maiti, Achyut Maity, D. V. Kuznetsov, P. Mondal, D. Senapati, RSC Advances **2016**, 6, 45279-45289.
8. Green silver nanoparticles for drug transport, bioactivities and a bacterium (*Bacillus subtilis*) mediated comparative nano-patterning feature, B. Dey, S. Mukherjee, N. Mukherjee, R. K. Mondal, B. Satpati, D. Senapati, S. P. Sinha Babu, RSC Advances **2016**, 6, 46573-46581.
9. Development of Triplet-Triplet Absorption Ruler: DNA- and Chromatin-Mediated Drug Molecule Release from Nanosurface. S. Daschakraborty, A. Sau, D. V. Kuznetsov, A. Banerjee, M. Bardhan, M. Bhattacharya, D. Dasgupta, S. Basu, D. Senapati, J. Phys. Chem. B **2016**, 120, 6872-6881 .
10. Hollow Gold Nanoprism as Highly Efficient "Single" Nanotransducer for Surface-Enhanced Raman Scattering Applications, B. Hazra, K. Das, S. Daschakraborty, M. S. Verma, M. M. Devi, N. K. Katiyar, K. Biswas, D. Senapati, M. Chandra, J. Phys. Chem. C **2016**, 120, 25548-25556.

11. Gold Nanoflowers and Gold Nanospheres as Labels in Lateral Flow Immunoassay of Procalcitonin, K. V. Serebrennikova, J. V. Samsonova, A. P. Osipov, D. Senapati, D. V. Kuznetsov, Nano Hybrids and Composites, 2017, 13, 47-53.

GUIDANCE/TEACHING

3 PhD Students (Ms. Maireyee Bhattacharyya, Joined in August-2013, Ms. Sudeshna DasChakraborty, Joined in August-2013, Sandip Kumar De, Joined in August-2015)

Post M.Sc. Biophysical Science: Spectroscopy & Nanomaterials; Nanobio materials and Chemical Physics

NATIONAL/INTERNATIONAL CONFERENCES

Invited Talks: 10 (Abroad: 4, National: 6)

RESEARCH AND DEVELOPMENT

- Nanomaterial synthesis, characterization and applications in Biomedicine & Biotechnology, Sensor Technology, Environmental Science and Renewable Energy Source
- Magnetic Nanomaterials and Polymer-based nano-composite
- Single molecule spectroscopy, Fluorescence and Raman Microscopy, Laser Spectroscopy and Dynamics, Photophysics and Photobiology
- Cyto- and geno-toxicity, Nanomedicine, Photothermal Lysis & Photothermal therapy.

National Level Academic Review

COMPUTATIONAL SCIENCE DIVISION

A Report for the period 2012-2017

Computational Science Division

Introduction

The Computational Science division was formed with two goals:

- a) Support the Institute with Computational resources, such as computer servers, Internet support, E-mail, E-governance, etc.
- b) Carry out computational research on Physics, Chemistry and Biology.

Some of our members are mostly engaged in computational research and some of our members are involved in developing, maintaining the computational infrastructure.

Present Staff

Prof. Dhananjay Bhattacharyya
Dr. Gautam Garai
Mr. Deepish Dey
Mr. Gautam Datta
Mr. Sumit Basu
Mr. Soumya Majumdar
Mr. Nandalal Sanpui
Mr. Subhendu Biswas

Present Students and Post-doctoral Fellows

Dr. Rakesh Kumar Mishra (DST-SERB RA)
Dr. Lakshmi Maganti (Institute RA)
Mr. Debasish Mukherjee (Finished Post M.Sc. in 2012)
Mr. Satyabrata Maiti (Finished Post M.Sc. in 2016)

Ph.D. Degree Awarded

Serial no.	Name of RF	Awarded in	University	Ph.D. Supervisor	Present location
1	Swati Panigrahi	2013	HBNI	D. Bhattacharyya	IIT-Hyderabad, India
2	Sukanya Halder	2014	University of Calcutta	D. Bhattacharyya	Kentucky, USA
3	Sanchita Mukherjee	2015	University of Calcutta	D. Bhattacharyya	IISER-K, India
4	Manas Mondal	2015	University of Calcutta	D. Bhattacharyya	Peking, China
5	Angana Ray	2016	University of Calcutta	D. Bhattacharyya	TIFR, Hyderabad, India

Development programs/projects:

The following projects were completed during 2012-2017:

- a. Migration and Enhancement of HA Cluster
- b. Modular Data Centre for Disaster Recovery (DR) Infrastructure
- c. Procurement and integration of NAC/UTM
- d. New Website of SINP
- e. Online Backup of Data for Administration
- f. VPN for Library Access
- g. HPC Installation
- h. Software development of few modules for E-governance

a. Migration and Enhancement of HA Cluster (DMZ Services):

The project involves migration of all the services (HTTP, SMTP, IMAPS, SSH, FTP, LDAP, DNS, Webmail etc.) and data to the new hardware and further enhancement to that. The solution also included the scope of DC and DR (Disaster Recovery) architecture, so that in case of a declared DR Scenario the DR setup can give critical service continuity to the users. As SINP does not have a campus at a geographically separate location, a location within our campus with electrical isolation was chosen to house the DR infrastructure. Storage (SAN) at both location and data replication at between the two sites was planned. Like before we planned to use Redhat HA Cluster Suite to handle High Availability between two nodes. The nodes can be in Active/Active or Active/Passive mode. There were provisions in the scope to also have a virtual system in place (using RHEV suite) and run some applications in that. The virtual infrastructure may grow in future to support Desktop and Server Virtualization Services to cater the need of other departments.

However, mainly due to the vast nature of the project, many customizations and other factors it took quite a while to have the migrated system in production. Eventually we have moved to a more of a Virtual environment with RHEV, with RedHat Enterprise Virtualization Manager to control the guest machines. Now there are more than 10 such hosts in the virtual environment running services like, WWW, Webmail, Mailstore, Mail Gateways, Name Servers, Gatekeeper (inward SSH access to SINP LAN), LDAP, IMAP/POP, Proxy, UFS etc. Virtualization benefits in better utilization of hardware resources, reduce Data Centre (DC) footprint, provides environment for testing, custom provisioning of hardware, reduce hardware vendor lock-in, extend the life of older applications. Recently we have moved to an open source solution for virtualization called oVirt.

The infrastructure continues to serve as a heart for email, web and other Internet services from 2013. However the DR infrastructure were fully utilized in 2016 with DR (Disaster Recover) System deployment followed by a DC-DR Drill. The DC-DR drill is actually a two part drill. The first part being migration of services from DC (#237) to DR(#3401) infrastructure. This involves switching off the primary site completely and run all the production services from DR site. A role reversal happens for all the connected LUNs of the SAN (Storage Area Network) pairs, the SAN of DR starts working as primary storage and stores all the production data. After few days of observation and running the production system on DR infrastructure a reverse drill

i.e. DR-DC Drill was conducted and storage and services were brought back to the DC infrastructure.

After the successful completion of the weeklong (21st to 26th July, 2016) DC-DR Drill, Dr. Sekhar Basu, Chairman AEC, along with a team of distinguished members and our Director inaugurated/visited the newly implemented DR Site. A poster session was also organised at the venue.

Our Director suggested that in future space may be provided at Belgachia Campus for hosting the DR site. Such an off-campus site would ensure complete electrical isolation of the two sites.

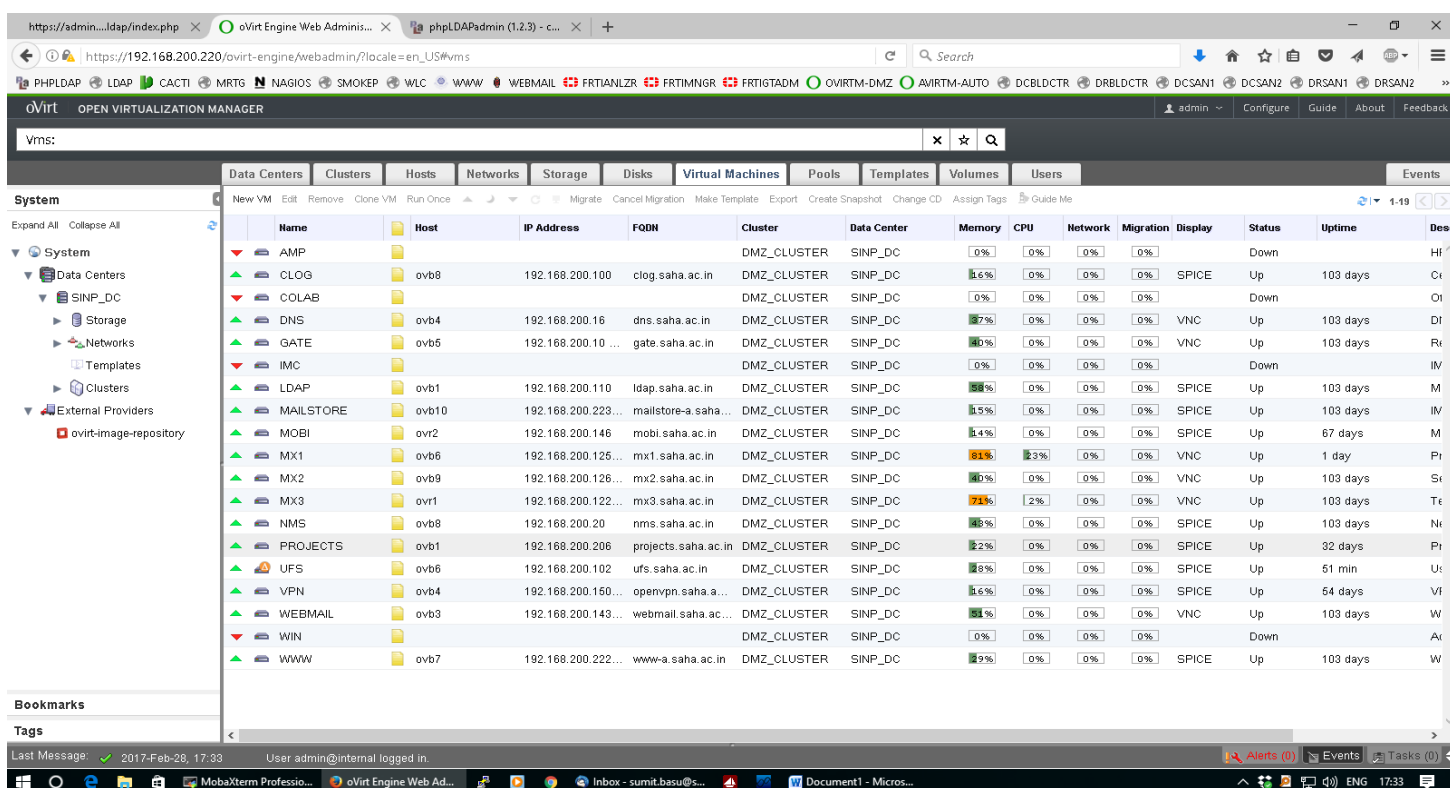


Fig: A Snapshot of Virtualization Environment with Guests (Virtual Machines)

b. Modular Data Centre for Disaster Recovery (DR) Infrastructure :

A project to have a Modular Data Centre (MDC), i.e. practically a Data Centre in one box was taken up to house the DR Infrastructure. A MDC has all the functionality of a formal DC, e.g. Precision Air Conditioning, UPS, Proper design of rack for air-flow etc. MDC architecture was also chosen for its movability. In future we would be able to shift the MDC to another campus to achieve better disaster recovery functionality and meet the guidelines of a proper DR setup. The MDC (Liebert XDFN) was operational from 2013. After Installation, DR servers and Storage along with network components/switches were installed in the rack of the MDC. MDC is now fully operational to house all the DR servers and equipment.

c. Perimeter and End Point Security and other Security Measures:

The Project of hardware Firewall/Unified Threat Management (UTM) system for perimeter and end points, the system was installed/configured was placed in the network replacing its software

counterpart. Other than basic Firewalling/Intrusion Prevention System, the UTM also works as a gateway agent for malware and spam control. Some of the benefits of the Unified Threat Management (UTM) system are the following:

- Hardware Gateway for high-speed Access (>1Gbps)
- Authenticated Access and hardware proxy
- Anti-malware Gateway
- Hardware Firewall
- High Availability of Firewall and Internet access
- Network Access Control and endpoint security

The division also takes care of the various IT security needs of the above installations and that of the Institute at large. The recommendations and guidelines of the CISAG (Computer & Information Security Advisory Group), DAE are followed and periodic exercises and assessments are carried out. As instructed by the CISAG (Chief Information Security Audit Group, DAE), initiatives were taken to form a group of technical members to help CISO in the domain of work.

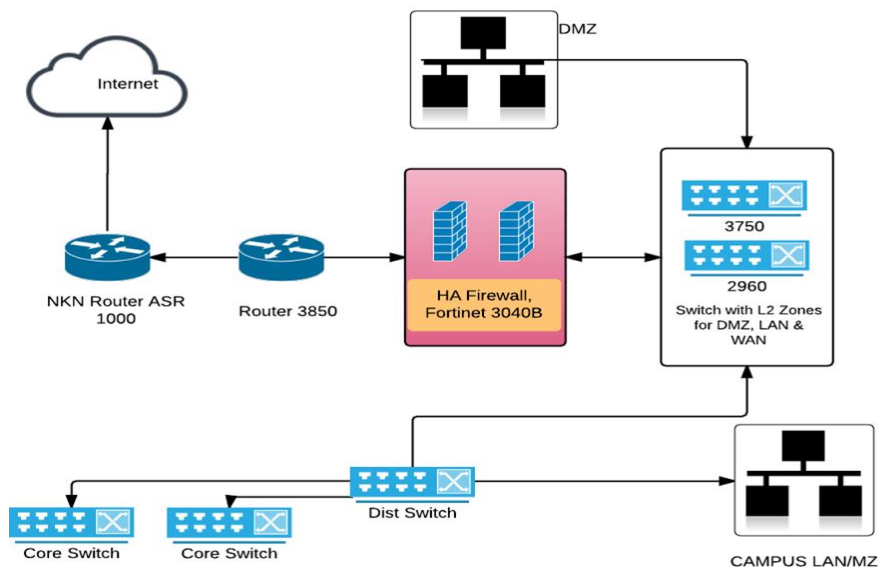


Fig: Perimeter Firewall integration in SINP Network

a. New Website of SINP

The project was completed in 2014. The objective was to use the modern technology & standard, homogeneous look and feel across all pages, to meet the UAT guidelines etc. The use of a modern Content Management System (CMS) and different templates for different category of pages were necessary part of the project. The new website of the Institute was inaugurated on the foundation day i.e. 11th Jan, 2014 by the Director. The project also involved delivery of many online applications accessed through an Application Portal. Backend LDAP installation was used for user authentication. Some unique features of the new website are given below:

- Content Management System, Template based page generation, Multilingual, Advanced Search, Text editor like WYSIWYG interface.
- 3 Tire access to website: Central, departmental and personal. Template for each section.

- Different template for centrally managed applications like Newsletter, Conference, Lectures and role based access control.
- Multimedia Gallery page, document uploading and maintenance by the user. Department-wise feedback, site-map, room locator.
- Application portal with authentication via central LDAP: Notice board, New Book Request (Library), Telephone Directory, Fault Reporting (AC/Electrical/Telephone/Network), Document Store, Dashboard, Auditorium Booking etc.

Many of the above functionalities are now running successfully for last 3 years. There are requests for many new applications which are getting developed in-house; some of these are inventory control, Guest House booking etc.

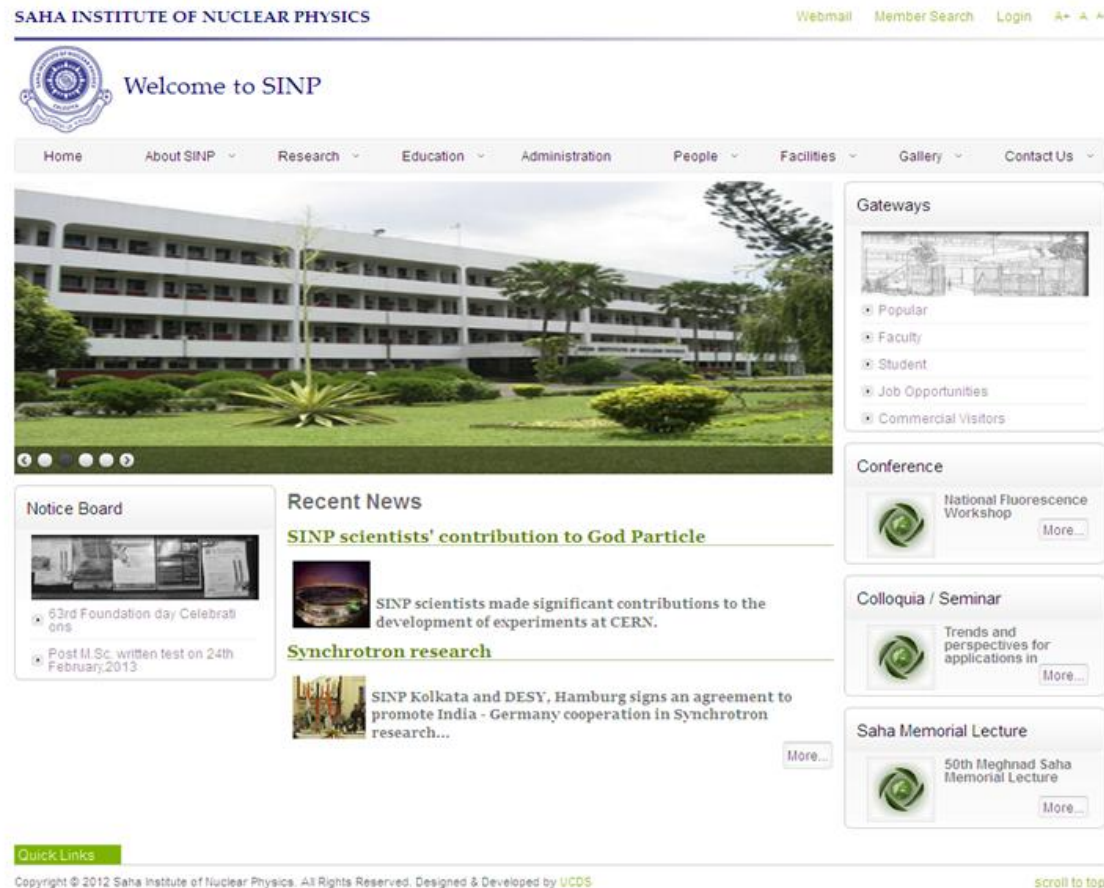


Fig: Landing Page (<http://www.saha.ac.in/>) of SINP Website

d. Online Backup of Data for Administration

Backup of data of the administrative sections of the Institute like the Director's office, Registrar's office and the Establishment office have also been started. The open source "Nextcloud" solution is being used as a cloud based data storage for providing this service to the users.

e. VPN for Library Access

VPN services using the perimeter UTM has been introduced for providing remote access to library services like online journal access and other facilities of SINP Library. Recently

VPN services for allowing remote users connectivity to internal LAN resources have also been introduced.

f. HPC Installation and support

In the division one HPC server (IBM Power 6) is maintained to cater the computational need of the institute as well as the members of the division. It consists of 8 sockets and each socket contains 4 cores. The main memory capacity is 8 GB/core and has huge hard disk space. A user can be allocated 50 GB space for the computation need in the environment of AIX Unix operation system with the availability of Fortran 90 and C compilers. The scientific software library like IMSL is also used by the users.

A six-node X86 cluster with 32 core AMD-opteron processors, 64 GB RAM on each node on CentOS Linux is also maintained by the Division for use of members of other division as well,

g. Software development of some modules for E-governance

The Guest-house booking, electricity consumption by staff staying in the housing complexes of SINP, etc. are now done by software developed by the divisional members. Few more are about to be completed soon.

Apart from the above projects the following are the major on-going projects:

- a. Network Refresh
- b. Data Centre For Room No. 235/3408
- c. RF-ID based e-Attendance
- d. CCTV Surveillance for SINP Campus
- e. Software Development for different modules of Office Automation
- f. GIGW Compliance Initiative, formation of different IT & User policies

Research Highlights:

Bioinformatics and Computational Sciences

Hybrid evolutionary algorithms were drawing significant attention for solving numerous real world problems. We had developed a new hybrid evolutionary approach for optimizing mathematical functions and Point Pattern Recognition (PPR) problems. The proposed method combined a global search genetic algorithm in a course-to-fine resolution space with a local (Tabu) search algorithm. Such hybridization enhanced the power of the search technique by virtue of inducing hill climbing and fast searching capabilities of Tabu search process. The approach can reach the global or near-global optimum for the functions in high dimensional space. Also, the hybrid method with grid based PPR technique had been applied for solving dot pattern shape matching and object matching represented as edge maps.

The evolutionary algorithm is based on computational models of natural selection and genetics. Genetic algorithms (GAs) are a particular class of evolutionary algorithms that use techniques inspired by evolutionary biology. Selection was one of the crucial operations in the GA process. We had studied the comparison of GA performance by varying the selection operator in solving a set of numerical functions. The selection strategy includes two traditional methods, tournament selection & Roulette wheel selection. We developed a Hybrid selection technique that basically combined the functionalities

of the two traditional selection methods.

Structural Bioinformatics and Molecular Modeling

Three-dimensional structures of RNA are known to be consisting of double helices with Watson-Crick base pairs. Several non Watson-Crick mismatch base pairs also appear in RNA quite frequently and quantum chemical studies had established their stability in gas-phase. Considering at least two hydrogen bonds are necessary to form a specific, stable and planar base pair, we found there is possibility of 124 types of non Watson-Crick base pairs among which about 100 types have been detected in the available structures of RNA. We have carried out quantum chemical studies of all these base pairs using DFT methods and a database was created.

We have developed a software to generate accurate model of a base pair using the six relative orientation parameters, Buckle, Open, Propeller, Stagger, Shear and Stretch, as suggested by IUPAC-IUB. This software can generate three-dimensional coordinates of double helical fragment also with such unusual base pairs. We have carried out extensive quantum chemical studies using Density Functional Theory with Dispersion correction on stacking interaction between successive base pairs in those double helical fragments. The structures predicted to have strongest stacking energy are seen to be quite similar to experimental structures for Watson-Crick base pair containing stretches. Thus we hope we can extend this method of stacking energy analysis to double helices containing non Watson-Crick base pairs as well.

We have done extensive molecular dynamics simulation studies to understand different features of DNA, such as melting behavior of polymeric DNA, molecular recognition of DNA sequences by protein through conformational selection mechanism, relative stabilities of telomeric DNA of different topology types, etc.

Planning for the Future:

We are in the process of installation of new Institute Local Area Network. This new network would have network backbone of 10Gbps connectivity from core switch to the distribution switches and at least 1Gbps connection up to the desktops and servers. This, augmented with the hardware firewall would immensely improve performance. Furthermore, this would allow us to share data within the campus as well as between different research organizations.

We have planned another interesting work on optimization for high dimensional mathematical functions by Artificial Bees Colony Optimization (ABCO). Our goal is to make the algorithm faster to achieve either better or similar results compared to the existing results. All these algorithms are applicable for single optimization problem. We have also started work on multi-optimization problems.

We are also developing an algorithm with Rough Set Clustering. It will be a useful classification technique for enhancing the accuracy of multi-dimensional data classification.

We are also working on gene prediction using the evolutionary algorithms for finding known genes in the large genomic sequences. We also like to develop efficient techniques for comprehensive study of next-generation sequencing.

Although structure, dynamics and stability of different non Watson-Crick base pairs are well studied, how they form double helical structure, which of them can form double helical structure, etc. are not known. We are planning to address these issues by performing model building studies of double helical fragments of different sequences including non Watson-Crick base pairs followed by energy refinement and molecular dynamics simulations.

There are huge number of three-dimensional structures of RNA solved by different experimental techniques, such as X-ray crystallography, Cryo-electron microscopy, etc. Many of these structures are of related molecules and hence these can also be considered as experimental ensemble. We are trying to classify the structures of RNA using their secondary structural features, such as appearance of a residue in double helix, loop, etc.

DHANANJAY BHATTACHARYYA, Professor H

DoB 10 July 1960

Phone 91 33 23370379 (ext: 2252)

E-mail: dhananjay.bhattacharyya@saha.ac.in

EDUCATION	1993: Ph.D. in Biophysics, Indian Institute of Science, Bangalore 1983: M.Sc. in Physics, University of Calcutta; 1 st Class 1981: B.Sc. Physics (major), University of Calcutta; 1 st Class
ACADEMIC POSITIONS	1996-....: Lecturer C, Biophysics Division, Saha Institute of Nuclear Physics ... to presently Professor H, Computational Science Division, 1993-1995: Visiting Fellow, Division of Computer Research and Technology, National Institutes of Health, Maryland, USA
TEACHING/ GUIDANCE	Regularly teach in Post M.Sc. Biophysical Science stream, subjects covered are Nucleic Acid Structure, Basic Statistics, Molecular Simulation Involved in Teaching at University of Calcutta, Bose Institute and West Bengal University of Technology as guest lecturer Ph.D. degree awarded (in the period 2012-2017) 5 ; Present students: 2
AREA(S) OF RESEARCH	My main interest is to understand structure-function relationship of biological macromolecules, especially of nucleic acids. In this regard we concentrate on available biomolecular structures solved by crystallography or NMR spectroscopy and look for different structural features, such as sequence dependent effect. We also carry out molecular dynamics simulation and <i>ab initio</i> quantum chemical calculations to understand structural stabilization of nucleic acid bases and recognition of nucleic acid by other ligands. We established molecular recognition through conformational selection model followed by induced fit mechanism for TATA box DNA – Tata box binding protein complex formation, using molecular dynamics simulations. In order to understand different structural features of nucleic acids, we have developed and are regularly upgrading few software, such as NUPARM, BPFIND, PyrHBFind, RNAHelix, etc. These are in public domain, can be downloaded from http://www.saha.ac.in/biop/bioinformatics/ and are widely used by other groups across the world. We have also created few databases of RNA structures and motifs and are distributed in public domain. Using some of these tools, we have classified structures of different non-canonical base pairs appearing in RNA crystal or NMR derived structures. We found from quantum chemical energy calculations that many of these basepairs, such as A:G H:S T, G:G H:W T, etc., are almost as stable as the canonical A:U W:W C basepair. The obvious question comes next is whether these non-Watson-Crick basepairs can form double helical structures similar to those formed by canonical ones. In order to address that we have carried out extensive analysis of stacking interaction energy between two basepairs considering effect of backbone in some simplistic way. We found that the recently developed Dispersion-Corrected Density Functional Theory (DFT) methods are capable to explain stacking preferences for most of the Watson- Crick basepaired dinucleotide steps and hence expect that the same method would be able to establish stacking features of the non-canonical basepairs.

In addition to biological macromolecules, we have also used DFT to understand different properties of some biologically important nano-particles, such as graphene, carbon-nanotube, gold nano-particle etc. We have shown importance of capping agents in formation and interaction of these nano particles, where the edge hydrogen atoms covalently bonded to the carbons of graphene show differential binding affinity with water depending on *cis* or *trans* edges. Similarly citrate groups, located at the edges of gold-nanoparticles were shown to have special interaction with quercetin like flavons.

PUBLICATION STATISTICS

Journals papers **39**; Conference Proceedings published in Journal: **2**

SELECTED PUBLICATIONS

- i) S. Panigrahi, A. Bhattacharya, S. Banerjee, D. Bhattacharyya (2012) Interaction of Nucleobases with Wrinkled Graphene Surface: Dispersion Corrected DFT and AFM Studies. *J. Phys. Chem. C* **116**: 4374
- ii) S. Halder and D. Bhattacharyya (2012) Structural Variations of Single and Tandem Mismatches in RNA Duplexes: A Joing MD Simulation and Crystal Structure Database Analysis. *J. Phys. Chem. B* **116**: 11845
- iii) S. Halder, D. Bhattacharyya (2013) RNA structure and dynamics: A base pairing perspective. *Prog. Biophys. Mol. Biol.* **113**: 264
- iv) P.K. Pingali, S. Halder, D. Mukherjee, S. Basu, R. Banerjee, D. Choudhury and D. Bhattacharyya (2014) Analysis of stacking overlap in nucleic acid structures: Algorithm and application. *J. Comp. Aided Mol. Des* **28**: 851.
- v) S. Mukherjee, S. Kundu, D. Bhattacharyya (2014) Temperature Effect on poly(dA).poly(dT): Molecular dynamics simulation studies of polymeric and oligomeric constructs. *J. Comput. Aided Mol. Des.* **28**: 735.
- vi) M. Mondal, D.Choudhury, J. Chakrabarti, D. Bhattacharyya (2014) Role of indirect readout mechanism in TATA box binding protein-DNA interaction. *J. Comp. Aided Mol. Des.* **29**: 283.
- vii) M. Mondal, S. Mukherjee, D. Bhattacharyya (2015) Stacking geometry for non-canonical G:U wobble base pair containing dinucleotide sequences in RNA: Dispersion-corrected DFT-D study. *Biopolymers* **103**: 328.
- viii) A. Ray, S. Panigrahi, D. Bhattacharyya (2015) A comparison of four different conformations adopted by human telomeric G-quadruplex using computer simulations. *Biopolymers* **105**: 83.
- ix) M. Mondal, S. Halder, J. Chakrabarti, D. Bhattacharyya (2016) Hybrid simulation approach incorporating microscopic interactions along with rigid body degrees of freedom for stacking between base pairs. *Biopolymers* **105**: 212
- x) D. Bhattacharyya, S. Halder, S. Basu, D. Mukherjee, P. Kumar, M. Bansal (2016) RNAHelix: Computational Modeling of Nucleic Acid Structures with Watson-Crick and Non-canonical Base Pairs. *J. Comp. Aided. Mol Des.* **31**: 219.

Name : **Gautam Garai**
Date of birth: December 12, 1964
Division : Computational Science Division

Present and Previous Employments :

Scientist 'G' at Saha Institute of Nuclear Physics from Feb., 2009 to till date.

Scientist 'F' at Saha Institute of Nuclear Physics from 2004-2009.

Scientist 'E' at Saha Institute of Nuclear Physics from 1999-2004.

Scientist 'D' at Saha Institute of Nuclear Physics from 1995-1999.

Scientist 'C' at Saha Institute of Nuclear Physics from 1992-1995.

Scientist 'B' at Saha Institute of Nuclear Physics from 1988-1992.

Assistant Systems Engineer at M.N. Dastur & Co. from 1987-1988.

Research Highlights :

In the field of Evolutionary Optimization it is necessary either to develop a new optimization algorithm or to modify the existing algorithm so that the old algorithm becomes faster. An effective hybrid genetic algorithm for solving clustering problems with multi-dimensional grid structure was developed. The algorithm is a combination of Genetic Algorithm (GA) and Tabu Search (TS) so that we can efficiently utilize the stochastic search ability of GA and the hill climbing as well as the local search capabilities of TS. Such hybridization helps to enhance the capability of both the search techniques and to reduce their disadvantages. The application of TS along with GA also greatly reduced the possibility of a stochastic search process to be trapped in a local optimal solution.

Similarly another efficient algorithm was developed by modifying the Ant Colony Optimization method for optimizing mathematical functions. The search process of the optimization approach is directed towards a region or a hypercube in a multidimensional space where the amount of pheromone deposited is maximum after a predefined number of iterations. The entire search area is initially divided into 2^n number of hypercubic quadrants where n is the dimension of the search space. Then the pheromone level of each quadrant is measured. Now, the search jumps to the region (new search area) of maximum pheromone level and restarts the search process in the new region. However, the search area of the new region is reduced compared to the previous search area. Thus, the search advances and jumps to a new search space (with a reduced search area) in several stages until the algorithm is converged.

In bioinformatics, the sequence alignment is an important and challenging task for sequence analysis. Biological sequences can be of variable lengths. We developed a new Genetic Algorithm (GA) based alignment technique for finding the best alignment score of a sequence pair in an optimized way. The pair of sequences is of equal or unequal length of DNA or protein sequences. The genetic based method named CPAGA (Cascaded Pairwise Alignment with Genetic Algorithm) was implemented into smaller subspaces by breaking a larger space. This was done by decomposing the sequence pair into multiple segments before the alignment.

Detection of important functional and/or structural elements and identifying their positions in a large eukaryotic genome is an active research area. Gene is an important functional and structural unit of DNA. The computation of gene prediction is essential for detailed genome annotation. We developed a new gene prediction technique based on Genetic Algorithm (GA) for determining the optimal positions of exons of a gene in a chromosome or genome. The correct identification of the coding and

non-coding regions are difficult and computationally demanding. The genetic-based method, named Gene Prediction with Genetic Algorithm (GPGA), reduced this problem by searching only one exon at a time instead of all exons along with its introns.

Teaching Courses Offered :

- Bioinformatics, PARL Programming Language and C Programming Language and its application in Bioinformatics courses to Post M.Sc.(Bio) students of SINP since 2012.

Research papers' reviewing of some International Journals :

a) Information Sciences, b) Pattern Recognition Journal, c) Journal of Pattern Recognition Research, d) Journal of Convergence Information Technology, e) IEEE Transactions on Systems, Man and Cybernetics : Part B, Cybernetics, f) IEEE Transactions on Cybernetics, g) IEEE Transactions on Evolutionary Computation, h) IEEE Transactions on Computational Biology and Bioinformatics, I) Journal OPSEARCH

Selected list of Publications :

- i) Biswanath Chaudhury and G. Garai, "A review on multiple sequence alignment from the perspective of genetic algorithm", Genomics, In Press.
- i) G. Garai and Biswanath Chaudhury, "A cascaded pairwise biomolecular sequence alignment technique using Evolutionary Algorithm", Information Sciences, 297(2015), pp. 118-139.
- ii) M. Basu P. Deb and G. Garai, "Hybrid of Particle Swarm Optimization and Simulated Annealing for multidimensional function optimization", Int. J. Information Tech., Vol. 20, No. 1, 2014, pp. 34-45.
- iii) G. Garai, Shayantan Debbarman and Tamalika Biswas, "An Efficient Ant Colony Optimization Algorithm for Function Optimization", Proc. of the IEEE Congress on Evolutionary Computation (CEC 2013), Cancun, Mexico, June 20-23, 2013, pp. 2345-2351.
- iv) G. Garai and B.B. Chaudhuri, "A novel hybrid Genetic Algorithm with Tabu search for optimizing multi-dimensional functions and point pattern recognition", Information Sciences, 221(2013), pp. 28-48.
- v) G. Garai and Biswanath Chaudhury, "A novel genetic approach for optimized biological sequence alignment", Journal of Biophysical Chemistry, Vol. 3. No. 2, 2012, pp. 201-205.

Complete list of publication from the Division:

(Highlighted authors are from the Division)

1. S. Kundu, S. Mukherjee, D. Bhattacharyya (2017) Melting of Polymeric DNA Double Helix at Elevated Temperature: A Molecular Dynamics Approach. *J. Mol. Model.* (in press).
2. A. Halder, R. Roy, D. Bhattacharyya, A. Mitra (2017) How does Mg²⁺ Modulate the RNA Folding Mechanism: A Case Study of the G:C W:W Trans Basepair. *Biophys. J* **113**: 1-13.
3. A. Mazumder, S. Batabyal, M. Mondal, T. Mondol, S. Choudhury, R. Ghosh, T. Chatterjee, D. Bhattacharyya, S. K. Pal, S. Roy (2017) Specific DNA Sequences Allosterically Enhance Protein-Protein Interaction in a Transcription Factor through Modulation of Protein Dynamics: Implications for Specificity of Gene Regulation. *Phys. Chem. Chem. Phys.*, **19**: 14781-14792.
4. D. Bhattacharyya, S. Halder, S. Basu, D. Mukherjee, P. Kumar, M. Bansal (2017) RNAHelix: Computational Modeling of Nucleic Acid Structures with Watson-Crick and Non-canonical Base Pairs. *J. Comp. Aided. Mol Des.* **31**: 219-235.
5. G. Naiya, P. Raha, M. Mondal, U. Pal, R. Saha, S. Chaudhuri, S. Batabyal, S.K. Pal, D. Bhattacharyya, N.C. Maiti, S. Roy (2016) Conformational Selection Underpins Recognition of Multiple DNA sequences by Proteins and Consequent Functional Actions. *Phys.Chem.Chem.Phys.* **18**: 21618-21628
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