

# National Level Academic Review

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*A Report for the period 2012-2017*

- 
- **CONDENSED MATTER PHYSICS (CMP) DIVISION**
    - **SURFACE PHYSICS AND MATERIAL SCIENCE (SPMS) DIVISION**

# **National Level Academic Review**

**Condensed Matter Physics Division (CMP Div.)**

**A Report for the Period 2012-2017**

## Present Staff

<b>Scientific (12)</b>	<b>Technical (8)</b>
Abhik Basu, Professor G	Anish Karmahapatra
Arti Garg, Associate Professor F	Arindam Chakrabarti
Barnana Pal, Professor F	Arun Kumar Pal
Bikas K Chakrabarti, Senior Professor I	Dhruba Jyoti Seth
Bilwadal Bandyopadhyay, Professor G	Kausik Das
Biswajit Karmakar, Associate Professor E	Papia Mondal
Chandan Mazumdar, Professor G	Prabir Das
Indranil Das, Senior Professor H	Sankari Chakraborty
Kalpataru Pradhan, Associate Professor E	
Prabhat Mandal, Senior Professor H	<b>Auxiliary (2)</b>
Pradeep Kumar Mohanty, Professor G	Jhantu Mallick
Sudhakar Yarlagadda, Senior Prof. H & Head	R Dubey
<b>Administrative (1)</b>	
Tapan Kumar Sarkar	

## Post Doctoral Fellows (2012-2017)

	<b>Name of RF</b>
1	Rima Pal
2	Biswanath Samanta Roy
3	Raghavendra K Rao
4	Papri Dasgupta
5	Analabha Roy
6	Koushik Sengupta
7	Anjan Chandra
8	Satyaki Kar
9	Arnab Chatterjee

## Present Research Fellows

	<b>Name of RF</b>	<b>Name of Ph D Supervisor</b>
1	Amit Chatterjee	Pradep K Mohanty
2	Amrita Ghosh	Sudhakar Yarlagadda
3	Apurba Dutta	Indranil Das
4	Arnab Kumar Pariari	Prabhat Mandal
5	Binita Mondal	Chandan Mazumdar
6	Gourab Majumder	Arti Garg
7	Mily Kundu	Chandan Mazumdar
8	Moumita Das	Prabhat Mandal
9	Moumita Nandi	Prabhat Mandal
10	Ratnadwip Singha	Prabhat Mandal
11	Ravindra Pankaj	Sudhakar Yarlagadda
12	Sabyasachi Nag	Arti Garg
13	Sanchayita Mondal	Chandan Mazumdar
14	Sanjib Banik	Indranil Das
15	Sanjukta Paul	Sudhakar Yarlagadda
16	Shubhankar Roy	Prabhat Mandal
17	Snehal Mandal	Indranil Das
18	Sourav Chakraborty	Kalpataru Pradhan
19	Sudipta Mondal	Chandan Mazumdar
20	Susmita Roy	Prabhat Mandal
21	Tirthankar Banerjee	Abhik Basu

## PhD Degree Awarded (2012-till date)

	<b>Name of RF</b>	<b>Awarded</b>	<b>Supervisor</b>	<b>Present Status</b>
1	Urna Basu	2013	Pradeep Kumar Mohanty	SISSA, Trieste, Italy
2	Prosenjit Sarkar	2013	Prabhat Mandal	Faculty, Serampore College
3	Sahinur Reja	2013	Sudhakar Yarlagadda	Post Doc, Indiana Univ. (USA)
4	Asim Ghosh	2014	Bikas K Chakrabarti	Post Doc. In Aalto Univ. of Technology, Helsinki
5	Debarshee Bagchi	2014	Pradeep Kumar Mohanty	CBPF, Rio, Brazil
6	Dilip Kumar Bhoi	2014	Prabhat Mandal	Post Doc fellow at Seoul National University
7	Niladri Sarkar	2015	Abhik Basu	Post Doc at MIPKs, Dresden, Germany

8	Rakesh Chatterjee	2015	Abhik Basu	Post Doc at ICF, UNAM, Mexico
9	Soymyajyoti Biswas	2015	Bikas K Chakrabarti	Post Doc. at Max Planck Inst , Goettingen
10	Mahashweta Basu	2015	Pradeep Kumar Mohanty	Univ. Maryland, USA
11	Sourish Bandyopadhyay	2015	Pradeep Kumar Mohanty	Met. Scientist, India
12	Arindam Midya	2015	Prabhat Mandal	Post Doc fellow at National University of Singapore
13	Nazir Khan	2015	Prabhat Mandal	Post Doc fellow at Augsburg University, Augsburg, Germany
14	Atanu Rajak	2016	Abhik Basu & Bikas K Chakrabarti	Post Doc at Bar-Ilan University, Ramat Gan, Israel
15	Kalipada Das	2016	Indranil Das	Assit Prof at S.A. Jaipuria Collage, Kolkata
16	Amit Dey	2016	Sudhakar Yarlagadda	Post Doc at Ben-Gurion University, Israel
17	Susmita Dhara	2017	Bilwadal Bandyopadhyay	Post Doc at IIT Bombay
18	Tapas Paramanik	2017	Indranil Das	Post Doc at IIT Kharagpur
19	Moumita Nandi	2017	Prabhat Mandal	
20	Sourav Kundu	2017	Sachindranath Karmakar & Prabhat Mandal	Post Doc at SNBNCBS, Kolkata
21	Manasi Ghosh	2013	Kajal Ghoshray	
22	Mayukh Majumder	2013	Kajal Ghoshray	Post Doc fellow at Augsburg University, Augsburg, Germany
23	Deep Talukdar	2013	Kamal Kumar Bardhan	Cryonano Labs Pvt Ltd
24	Paramita Dutta	2015	Sachindranath Karmakar	Post Doc at IoP, Bhubaneswar
25	Moumita Dey	2015	Sachindranath Karmakar	Asst Prof at Adamas University

### PhD Thesis Submitted

	Name of RF	Submitted	Supervisor	Present Status
1	Rajeswari Roychowdhury	2016	Bilwadal Bandyopadhyay	
2	Santanu Pakhira	2017	Chandan Mazumdar	
3	Bijoy Daga	2017	Pradeep Kumar Mohanty	Post Doc at IMSc, Chennai
4	Srilekha Saha	2017	Sachindranath Karmakar & Prabhat Mandal	

## Experimental & Theoretical Facilities in CMP Division:

### 1. Sample preparation facilities:

- a. Image Furnace for Single Crystal growth
- b. Pulsed Laser Deposition System
- c. Argon Arc Furnace
- d. Ultra-High Vacuum Deposition System
- e. Clean Room Processing for Device Fabrication

### 2. Characterization Facilities:

- a. Powder X-Ray Diffraction Facility
- b. Atomic Force Microscopy

### 3. Measurement Facilities:

- a. SQUID-VSM Magnetic Measurement Facility
- b. Physical Properties Measurement Systems- 2.
- c. Solid State NMR System
- d. High Temperature VSM System
- e. Magnetotransport Measurement Facilities- 2.
- f. P-E loop Tracer System

### 4. Computation Facility:

500 node cluster

## Achievements (2012-2017):

### **Publications: More than 200**

**Includes:** 3 PRL, 1 Nature Commun., 1 PNAS, 29 PRB, 13 APL, 9 Sc. Rep., 25 PRE, 4 EPL, and papers in other reputed journals (RSC, JPCC, Plos ONE, NJP, etc.)

**Reviews:** 1 RMP + 1 Phys Rep. + 1 EPJ Spl.

**Books:** 6 (Oxford, 3 Cambridge, Springer, Wiley)

**Invited talks:** Many national and international conferences/workshops.

*For details, see individual CVs.*

## Research Interests:

**Abhik Basu:** (i) hydrodynamic approaches to driven or active membranes; (ii) nonequilibrium dynamics of topological defects and associated phase transitions; (iii) statistical physics applications in hydrodynamic turbulence and related topics; (iv) exclusion processes, conservation laws and finite resources; and (v) theories for active smectic phases.

**Arti Garg:** interested in the broad area of condensed matter physics, especially in role of interactions and disorder in condensed matter systems. For example, localization in presence of both interactions and disorder, that is, many-body localization, effect of disorder and interactions in graphene, the role of interactions in band-insulators, etc. Also interested in the field of spintronics, looking for new mechanisms for interaction driven half-metallicity and transport in general in condensed matter systems.

**Barnana Pal:** interested in Fourier acoustics for precision measurement. Acoustical methods play a major role in present day science and technology and improvement in precision of measurement of wave propagation parameters, viz., the velocity  $v$  and attenuation  $\alpha$ , require further research on the most popular methods in use. Though reasonably good precision is obtained for velocity measurement, one finds it too difficult to obtain a dependable value for  $\alpha$ , which is very sensitive to the experimental conditions. Theoretical analysis indicates that the reason is an inherent property of the technique itself and a possible solution in this regard is the application of Fourier transform method. Developing a Fourier Transform Pulse-Echo technique for precision measurement of  $\alpha$  is the current topic of research in the Ultrasonic Lab of CMP Division.

**Bikas K Chakrabarti:** (i) Quantum Spin Glasses & Quantum Annealing ; (ii) Statical Physics of Fracture ; and (iii) Physics Models of Society: Econophysics.

**Bilwadal Bandyopadhyay:** Preparation, characterization and study of magnetic properties of bimetallic magnetic nanoparticles.

**Biswajit Karmakar:** interests are optical spectroscopy and electronic transport study of semiconductor nanostructures and quantum Hall systems at dilution fridge temperatures under a high magnetic field. Using these studies we explore the correlated states of the semiconductor quantum structures and their physical properties in view of implication on quantum technology.

**Chandan Mazumdar:** primary research interest is the study of structural, magnetic and superconducting properties of new intermetallic materials that have prospects of exhibiting diverse kind of novel phenomena. Various tools, viz., different laboratory based facilities, as well as large experimental facilities like neutron and synchrotron centers, are being utilized to study the physical properties of those materials.

**Indranil Das:** synthesis of Advance Energy Materials & Hybrid Nano-Structure using PLD for superior magnetocaloric, electrocaloric, multiferroic, thermoelectric properties. Device structure fabrication for Spintronics & studies on Spin Caloric Transport, large local/nonlocal magnetoresistance. Mirror coating for LIGO India using dual ion beam sputtering deposition.

**Kalpataru Pradhan:** (i) physics at the interface of ferromagnetic and insulating layers in transition metal oxides.; and (ii) disorder induced magnetism in Graphene.

**Prabhat Mandal:** We are interested in investigating novel electronic properties of 3D topological insulator and Dirac/Weyl systems through magneto-transport and other techniques. First, we plan to grow high quality single crystals of completely new and theoretically predicted topological materials. The electronic properties of these crystals will be studied at very high magnetic field and low temperature down to mili-Kelvin to observe novel phenomena as it approaches quantum limit regime.

**Pradeep Kumar Mohanty:** have been working towards developing a formulation of non-equilibrium thermodynamics; a general formalism appears to be far from reach but we aim at characterizing a class of exactly solvable no-equilibrium models and apply the concepts developed there to understand the thermodynamics behavior of generic non-equilibrium systems. Research interests also include non-equilibrium phase transition, percolation, self organized criticality, hyper-uniformity etc. Besides this, working on biological networks, in particular miRNA or protein-interaction networks, to understand genetic aspects of certain disease, like spinal cord injury, cancer, Huntington disease etc.

**Sudhakar Yarlagadda:** Strong-weak duality treatment in condensed matter; supersolidity in hard-core-boson systems; Hubbard-Holstein model; analyze systems with strong cooperative electron-phonon interaction; oxide devices (qubits, heterostructures) as replacement for semiconductor devices; correlation between battery performance and basic physics of Li batteries; entanglement and decoherence in spin systems.

**Collaboration:** Active intra-division, inter-division, inter- institutions (National & International).

***For Research Highlights and Future Directions, see individual CVs.***



## ABHIK BASU

**PhD Student:** (i) Dr Niladri Sarkar (2015) – now at MPIPKS, Dresden, Germany (ii) Dr Rakesh Chatterjee (2015) – now at ICF, UNAM, Mexico, (iii) Dr Atanu Rajak (jointly with Prof. Bikas K Chakrabarti) (2016) – now at Bar-Ilan University, Ramat Gan, Israel, (iv) Mr. Tirthankar Banerjee (continuing).

### LIST OF PUBLICATIONS : 2012 - 2017

1. N. Sarkar and A. Basu, Instabilities and diffusion in a hydrodynamic model of a fluid membrane coupled to a thin active fluid layer, Eur. Phys. J. E 35, 115 (2012).
2. A. Basu and J. K. Bhattacharjee, Fluctuating hydrodynamics and turbulence in a rotating fluid: Universal properties, Phys. Rev. E 85, 026311 (2012).
3. N. Sarkar and A. Basu, Continuous Universality in nonequilibrium relaxational dynamics of  $O(2)$  symmetric systems, Phys. Rev. E 85, 021113 (2012).
4. A. Basu, J.-F. Joanny, F. Jülicher and J. Prost, Anomalous diffusion in thin active films, New J. Phys. 14, 115001 (2012).
5. N. Sarkar and A. Basu, Active to absorbing state phase transition in the presence of a fluctuating environment: Weak and strong dynamic scaling, Phys. Rev. E 86, 021122 (2012).
6. N. Sarkar and A. Basu, Phase transitions and continuously variable scaling in a chiral quenched disordered model, Phys. Rev. E 87, 032118 (2013).
7. R. Chatterjee, A. K. Chandra, and A. Basu, Phase transition and phase coexistence in coupled rings with driven exclusion processes, Phys. Rev. E 87, 032157 (2013).
8. N. Sarkar and A. Basu, Phases and fluctuations in a model for asymmetric inhomogeneous fluid membranes, Phys. Rev. E 88, 042106 (2013).
9. N. Sarkar, A. Basu, J. K. Bhattacharjee and A. K. Ray, Acoustic horizons in steady spherically symmetric nuclear fluid flows, Phys. Rev. C 88, 055205 (2013).
10. N. Sarkar and A. Basu, Generic instabilities in a fluid membrane coupled

to a thin layer of ordered active polar fluid, *Eur. Phys. J E* 36, 86 (2013).

11. A. Basu, A. Naji and R. Pandit, Structure-function hierarchies and von Kármán-Howarth relations for turbulence in magnetohydrodynamical equations, *Phys. Rev. E* 89, 012117 (2014).

12. N. Sarkar and A. Basu, Active to absorbing state phase transition in the presence of a fluctuating environment: Feedback and universality, *J. Stat. Mech.* Online at [stacks.iop.org/JSTAT/2014/P08016](http://stacks.iop.org/JSTAT/2014/P08016) (2014).

13. N. Sarkar and A. Basu, Nonequilibrium steady states in asymmetric exclusion processes on a ring with bottlenecks, *Phys. Rev. E* 90, 022109 (2014).

14. R. Chatterjee, A. K. Chandra and A. Basu, Asymmetric exclusion processes on a closed network with bottlenecks, *J. Stat. Mech.*, Online at [stacks.iop.org/JSTAT/2015/P01012](http://stacks.iop.org/JSTAT/2015/P01012) (2015).

15. T Banerjee and A Basu, Thermal fluctuations and stiffening of symmetric heterogeneous fluid membranes, *Phys. Rev. E*, 91, 012119 (2015).

16. T Banerjee, N Sarkar and A Basu, Generic nonequilibrium steady states in an exclusion process on an inhomogeneous ring, *J. Stat. Mech.*, Online at [stacks.iop.org/JSTAT/2015/P01024](http://stacks.iop.org/JSTAT/2015/P01024) (2015).

17. T Banerjee, A K Chandra and A Basu, Phase coexistence and particle non-conservation in a closed asymmetric exclusion process with inhomogeneities, *Phys. Rev. E* 92, 022121 (2015).

18. N. Sarkar and A. Basu, Phase transitions and membrane stiffness in a class of asymmetric heterogeneous fluid membranes, *J. Stat. Mech.*, P08023 (2015).

19. N. Sarkar and A. Basu, Role of interfacial friction for flow instabilities in a thin polar ordered active fluid layer, *Phys. Rev. E* 92, 052306 (2015).

20. T Banerjee, N Sarkar and A Basu, Phase transitions and order in two-dimensional generalized nonlinear  $\sigma$ -models, *Phys. Rev. E* 92, 062133 (2015).

21. A. K. Ray, N. Sarkar, A. Basu and J. K. Bhattacharjee, Spontaneous azimuthal breakout and instability at the circular hydraulic jump, *arXiv:1506.05924* (2015).

22. T. Banerjee and A. Basu, Active processes make lipid membranes either flat or crumpled, *arXiv:1512.03418* (2015).

23. B. Daga, S. Mondal, A. K. Chandra, T. Banerjee and A. Basu, Phase coexistence in a closed inhomogeneous asymmetric exclusion process with particle attachments and detachments, *Phys. Rev. E* 95, 012113 (2017).

24. P. Dolai, A. Basu, A. Simha, Universal spatiotemporal scaling of distortions in a drifting lattice, *Phys. Rev. E* 95, 052115 (2017).
25. A. K. Chandra and A. Basu, Diffusion Controlled Model of Opinion Dynamics, *Rep. Adv. Phys. Sci.* 01, 1740008 (2017).
26. T. Banerjee and A. Basu, Active synchronization and ordering of coupled oscillators, accepted for publication in *Phys. Rev. E* (2017).
27. T. Banerjee, N. Sarkar, J. Toner and A. Basu, Rolled up, flat or crumpled: phases of asymmetric tethered membranes, manuscript in preparation (2017); preliminary version available at arXiv:1610.01992.

### Research highlight:

- Studies on active fluids, or active matters: Active fluids, or active matters are a class of generic coarse-grained theories proposed to describe wide variety of phenomena, ranging of cytoskeletal dynamics in the cells of developed animals, flocks of birds and schools of fishes. From nonequilibrium statistical mechanics point of views, all of these are systems with orientable degrees of freedom and hence extend the theories of equilibrium liquid crystals to nonequilibrium domains. Of particular interests to us are the dynamics of chiral active systems, dynamics of isolated biofilaments (e.g., microtubules and DNA strands) in an ordered active fluid and stochastic dynamics of active permeating fluids in the bulk or in the form of a thin film.
- Studies on biomembranes: Examples include soft or lipid membranes (e.g., cell membranes of eukaryotic cells) and tethered or stiff membranes (e.g., red blood cell membranes). Questions of interests are out of equilibrium miscibility phase transitions, possibilities of long-range orientational order in driven membranes, and the nature of crumpling and crinkling transitions.
- Theoretical studies on homogeneous fluid turbulence and related systems. We are interested in elucidating the multiscaling, or anomalous scaling of the relevant structure functions.
- Studies of simple equilibrium and nonequilibrium statistical mechanics models.
- Field theory applications in statistical mechanics and dynamics.
- Hydrodynamic descriptions for models of social dynamics.
- Hydrodynamic descriptions of fracture.

**External research support:** (i) Max-Planck-Society (Germany) – DST (India) Partner Group scheme (2009 – 2014), (ii) Alexander von Humboldt Research Group Linkage Programme scheme (2016 – 2019).

## ARTI GARG

**Designation:** Associate Professor 'F'  
**Office Address:** Condensed Matter Physics Division, SINP  
**Email:** arti.garg@saha.ac.in  
**Date of Birth:** 30<sup>th</sup> July 1977  
**Nationality:** Indian

### Education

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- Ph. D. in Physics, Tata Institute of Fundamental Research, Mumbai (2006)  
Thesis title: “ *Strongly Correlated Systems: Metal-Insulator transitions and Superconductors*”  
*Thesis Supervisor: Prof. Mohit Randeria*
- M. Sc. in Physics, University of Delhi, India (1999)
- B. Sc. in Physics, University of Delhi, India (1997)

### Employment

1. Postdoctoral fellow at Technion-Israel Institute of Technology, Haifa, Israel (October 2006 - August 2009).
  2. Postdoctoral fellow at University of California, Santa Cruz, CA, USA (September 2009 - June 2011).
  3. Associate Professor 'E' at Saha Institute of Nuclear Physics, Kolkata, India (August 2011- June 2016).
  4. Associate Professor 'F' at Saha Institute of Nuclear Physics, Kolkata, India (July 2016-).
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### Teaching Experience

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1. Computational Methods for Quantum Many Body Systems (1Dec 2011 to 31st March 2012)
2. Advanced Condensed Matter Physics (1st April 2014-31st July 2014)
3. Numerical Methods and Algorithms (August 2015 to 31st Nov 2015) with Kalpataru Pradhan

4. Advanced Condensed Matter Physics (1st Dec 2015 to 31st March 2016) with Kalpataru Pradhan.
5. Advanced Condensed Matter Physics-II(1st April 2016-31July 2016) shared with Kalpataru Pradhan.
6. Advanced Condensed Matter Physics -I (1st Dec 2016-30th March 2017).

## Supervision of Research Projects

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- Post-M.Sc. project by Ms. Anwesha Chattopadhyay (Dec 2016 – present).
- Post-M.Sc. project by Mr. Sabyasachi Nag (Dec, 2011 – July 2012).
- Post-M.Sc. project by Mr. Gourab Majumder (Dec. 2011 – July, 2012).
- Ph.D. Supervisor for Mr. Sabyasachi Nag and Gourab Majumder

## Research Interests

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I am interested in the broad area of condensed matter physics, especially in {it strongly correlated and disordered systems} e.g., many body localization, the effect of disorder on strongly correlated d-wave superconducting state of high  $T_c$  superconductors, effect of disorder in graphene, the role of interactions in band-insulators, interaction-induced metallic and half-metallic phases. I am also interested in transport in strongly correlated systems such as Wiedemann-Franz law in Luttinger liquids and transport in hard core Bosons.

## List of Publications Since 2012

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1. *Doping a correlated band insulator: a new route to half-metallicity*, **Arti Garg**, H. R. Krishnamurthy, and Mohit Randeria, *Phys. Rev. Lett.* **112**, 106406 (2014).
2. *Phase diagram of the half-filled ionic Hubbard model*, Soumen Bag, **Arti Garg** and H. R. Krishnamurthy, *Phys. Rev. B* **91**, 235108 (2015).
3. *Nature of Single Particle States in Disordered Graphene*, Sabyasachi Nag, **Arti Garg** and T. V. Ramakrishnan, *Phys. Rev. B* **93**, 235426 (2016).
4. *Drude weight in hard core Boson systems: possibility of a finite temperature Bose-metal*, Gourab Majumder and **Arti Garg**, *Phys. Rev. B* **94**, 134508 (2016).

5. Many-body mobility edges in an one-dimensional model of interacting fermions, *Sabyasachi Nag and Arti Garg*, Arxiv: 1701.00236 (Under Review)

### **Presentations in Conferences Since 2012**

1. "Correlations and Disorder in Quantum and Classical Systems" held at ICTS (Bengaluru) (29th May 2017 to 2nd June 2017). \

**Title of the talk:** "Many-body mobility edges in a one-dimensional model of interacting fermions"

2. Invited talk at Indo-US bilateral workshop on "Physics and Chemistry of Oxides: Theory meets experiments" (PCOTE17, 3rd Jan 2017 to 5th Jan 2017).

3. "Quantum Disordered Systems" at Institute of Mathematical Science (IMSc), Chennai, from 24-29 February 2016.

**Title of the talk:** "Nature of Single-particle states in disordered graphene".

4. "Condensed Matter Days 2014" at University of Calcutta, from 27-29 August 2014.

**Title of the Talk:** "Doping a correlated band insulator: a new route to half-metallicity".

5. "Physics and Chemistry of Materials: Computation and Experiments" held at S. N. Bose National Center for Basic Sciences, Kolkata from 24-25 February 2014.

**Title of the Talk:** "Semi-metal to Anderson Insulator transition in disordered graphene".

6. "Strongly correlated systems: From models to materials" organised by the International Center for Theoretical Sciences (ICTS) at Indian Institute of Sciences, Bangalore from 10-13 January 2014.

**Title:** "Doping a correlated band insulator: a new route to half-metallicity"

### **Other Invited Talks since 2012**

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1. Invited colloquium talk at Physics department, Presidency University, Kolkata on 29th March 2017.

Title of talk "What is many-body localization?"

2. Invited talk at School of physical sciences, Jawaharlal Nehru University on 5th Dec 2016.

Title of the talk "Nature of single particle states in disordered graphene"

3. Talk at Indian Association for Cultivation of Sciences (IACS), Kolkata on 22ND September 2015.

Title: "Nature of Single Particle States in Disordered Graphene".

4. Talk at S. N. Bose National Center for Basic Sciences, Kolkata on 10th March 2015.

Title: "Doping a correlated band insulator: a new route to half-metallicity".

5. Talk at Indian Institute of Science Education and Research (IISER)-Kolkata on 5th March 2014.

Title: "Doping a correlated band insulator: a new route to half-metallicity".

## Research Highlights

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My recent research has been related to the role of interactions in band insulators, interplay of interactions and disorder to look for possibilities of many body localization, effect of disorder in graphene, transport in strongly correlated materials etc. Below I give a brief description of these works.

### 1. Many-body localization of interacting fermions in an aperiodic potential:

According to the seminal work by Anderson, in a non-interacting disordered system quantum-interference among impurity scattered paths might result in a diffusion-less situation due to localization. The question of immense interest, that has remained unanswered for decades after Anderson's work, is what happens to Anderson localization when both disorder and interactions are present in a system. Recently Basko et. al.(Ann. Phys. **321**), 1126 (2006)

based on their perturbative treatment of interactions have established that if all the single particle states are localized in the non interacting system, then localization can survive even in interacting system for weak enough interactions resulting in a many body localized (MBL) phase. In this work, we ask the question what is the role of interactions in situations where the non interacting system has single particle mobility edge(ME) which separates the localized states from the extended states. This is an important unanswered question in the field as not even a perturbative treatment of interactions has been done for this case yet. We explore effects of interactions among spin-less fermions in an aperiodic potential which has single particle mobility edges in 1-d in the absence of interactions (S. D. Sarma et. al Phys. Rev. B **41**), 5544 (1990)).

Though according to the conventional wisdom, interactions should hybridise localized and extended states and the interacting system in such cases should not have any localization, we demonstrate based on exact diagonalisation study, that even in the presence of interactions some of the many body states remain localized resulting in many-body mobility edges. We also provide a comparison between various characterizations and diagnostic tools of MBL phase namely, energy level statistics, participation ratio in Fock space, Shannon entropy, entanglement entropy and eigenstate thermalisation hypothesis.

This work is done with my student Sabyasachi Nag at SINP.

Reference: arxiv: 1701.00236 (Under Review)

### 2. Drude weight in hard core Boson systems: possibility of a finite temperature ideal conductor:

Typical phases which are realized in lattice boson models are superfluid and insulating phases. In some cases coexistence of charge density wave (CDW) order and super fluidity, which is known as the supersolid (SS) phase, is also seen.

Most challenging phase, which is rarely seen, is gap less, compressible "Bose-Metal" phase which breaks no symmetry whatsoever. There are very few examples of studies where "Bose-Metal" phase has been realized. We define a Bose metal/ideal conductor to be the one with non zero Drude weight  $D$  but a zero superfluid stiffness  $\rho_s$  while a superfluid (SF) phase is the one in which both  $\rho_s$  and  $D$  are non-zero. In an insulating phase, e.g. in the CDW ordered phase, both  $\rho_s = D = 0$ . Here  $D$  is the delta function part of the charge conductivity  $\sigma(\omega) = D\delta(\omega) + \sigma_{reg}(\omega)$  and  $\rho_s$  is given by the curvature

of the thermodynamic limit of the free energy ( $\sim d^2\{F\}/d\phi^2$ ) with respect to a twist in boundary conditions ( $\phi$ ). In this context, it is interesting to consider non-interacting Bose gas in one and two dimensions. In this case, at any finite temperature  $\rho_s=0$  but since the current operator commutes with the Hamiltonian, the Drude weight remains finite at finite temperature. Therefore, non-interacting bosons in one and two dimensions at finite temperature are "trivial" examples of a Bose ideal conductors.

In this work we study the Drude weight in a model of hard core bosons (HCB), with nearest neighbour and next nearest neighbour hopping and repulsion terms, on 2D square lattice and cubic lattice. We calculated the Drude weight in the SF, insulating and SS phase of this model using stochastic series expansion method. We demonstrate from our numerical calculations that the normal phase of HCB's in two dimensions can be a Bose-metal (an ideal conductor). In the two dimensional case, for the SF ground state, the superfluid stiffness drops to zero in the thermodynamic limit with a Kosterlitz-Thouless type transition at  $T_{KT}$ . We found that though the Drude weight is equal to the stiffness below  $T_{KT}$  as expected, surprisingly it remains finite even for temperatures above  $T_{KT}$  indicating the presence of a Bose-metal or an ideal Bose conductor in the normal phase of this two-dimensional SF. On the other hand, in three dimensions, where the superfluid transition is accompanied by the appearance of true long-range order and the superfluid stiffness goes to zero with a continuous transition at  $T_c$ , we found that the Drude weight goes to zero at  $T_c$ . In a 2D supersolid phase, where the charge density wave (CDW) order coexists with the superfluidity, and transition temperature for CDW order is larger than  $T_{KT}$ , the Drude weight remains equal to the superfluid stiffness at all temperatures and goes to zero at  $T_{KT}$ .

This work is with my student Gourab Majumder.

Reference: Phys. Rev. B **94**, 134508 (2016).

**3. Effect of disorder in graphene:** Graphene, a two dimensional form of carbon, is different from conventional two dimensional electron systems in many ways. Although there are experimental techniques

to produce graphene with high crystalline quality, disorder is inevitable. According to the scaling theory of localization, any small amount of disorder should localize states in graphene, like in any other two dimensional

electron system. Graphene can be described by a tight-binding model on a 2D honeycomb lattice and the energy dispersion is linear in momentum near the Fermi points at half-filling resulting in Dirac like quasi-particles. It is well known that the Dirac states in graphene evade Anderson localization in the presence of weak long range charge impurities. Only short range impurities or very strong long range impurities, either of which can cause scattering from one Dirac valley to another, show weak localization correction to conductivity rather than weak-anti localization. But the nature of single particle states away from the Dirac point has not been explored in detail so far. Does a higher energy state, away from the Dirac point, get localized in the presence of an infinitesimal strength of disorder, as expected for a conventional 2D system from the scaling theory of localization or does it evade localization like a Dirac state? In this work we focus on these questions in detail.

We analyse the nature of the single particle states, away from the Dirac point, in the presence of long-range charge impurities in a tight-binding model for electrons on a two-dimensional honeycomb lattice which is of direct relevance for graphene. We demonstrated that not only the Dirac state but all the single particle states remain extended in the presence of weak long range impurities due to generic anti localization effects and prohibited backscattering events. This is



because the nature of low energy Hamiltonian and the wave functions are basically of the same nature as for the Dirac states. The wave function for any energy state  $E$  picks up a phase  $\pi$  under a backscattering process which is thus suppressed. A threshold strength  $V_{th}$  of disorder is required to localize a state with energy  $E$  since the random potential needs to scatter an electron from point  $\vec{k}$  on an equal energy contour of energy  $E$  to point  $-\vec{k}$  on it. Therefore, though states near the band center remain extended for weak to intermediate values of disorder strength, states near the band edge show extended nature only for weak disorder. We do see clear indications of this in the analysis of inverse participation ratio (IPR), charge conductivity and the generalized diffusion coefficient  $D_E(t)$ .

This work is in collaboration with my student Sabyasachi Nag (SINP) and T. V. Ramakrishnan (IISc, Bangalore and B. H. U.)}, Reference : Phys. Rev. B **93**, 235426 (2016).

**4. Interaction driven half-metallic phase:** Turning on strong correlations in a normal metallic system results in interesting phases like antiferromagnetic Mott Insulator, high  $T_c$  superconductor, pseudogap phase etc. But the role of strong correlations in a band insulator has not been explored much. We study the effect of strong correlations in a band insulator and show a novel interaction driven route to the formation of ferrimagnetic Half metal phase upon doping a correlated band insulator. Half metals is an interesting class of materials in which electrons with one spin direction behave as a metal and electrons with the opposite spin direction behave as an insulator. Half metals are ideal for spintronics as it can generate spin-polarized current.

To study the effect of correlations in a band insulator, we studied a variant of the Hubbard model with a staggered potential on sites of a bipartite lattice which makes the system at half filling for Hubbard  $U=0$  a band insulator (BI). This model is also known as the ionic Hubbard model. At half-filling, as  $U$  increases, the system undergoes a first order phase transition from paramagnetic BI to AFM Mott insulator (MI). Due to the staggered potential, AF MI has different spectral gaps for the two spin components and upon doping with holes this system becomes a ferrimagnetic half-metal (HM). The HM phase survives for a wide range of doping and  $U$  values.

The e-e interaction driven mechanism for half-metallicity we proposed in this work, has now been realised recently in some class of materials by Tanusri Saha-Dasgupta and co-workers (Scientific Reports, vol 5, 15010 (2015)).

This work is in collaboration with H.~R.~ Krishnamurthy (Indian Institute of Sciences, Bangalore) and Mohit Randeria (The Ohio State University, USA.)}

Reference : Phys. Rev. Lett. **112**, 106406 (2014).

**5. Phase diagram of Ionic Hubbard model:** We study the effect of strong correlations in a band insulator using the ionic Hubbard model (IHM) which is an interesting extension of the regular Hubbard model. The physics of the IHM is governed by the competition between the staggered ionic potential  $\Delta$  and the on-site Hubbard  $U$ . We find that at half filling for a finite  $\Delta$  the system is a band insulator (BI) at  $U=0$ . As we turn on the onsite repulsion  $U$  in this BI, first an antiferromagnetic (AFM) order sets in via a first order transition at  $U = U_{AF}$ . This is followed by a quantum phase transition to novel half-metallic AFM phase at  $U = U_{HM} > U_{AF}$ . For still larger values of  $U$ , this system becomes an AFM insulator.

We study this model within dynamical mean field theory using two different impurity solvers, namely. iterative perturbation theory (IPT) and continuous time quantum Monte Carlo (CTQMC). Up to moderately strong values of  $U$  (e.g.,  $U/t = 6.0$  for  $\Delta = 1.0t$ ), the IPT captures the effects of electron-electron correlations quite well, and yields essentially the same results as

CTQMC. But in the extremely correlated regime, where  $U \gg \Delta, t$ , DMFT+IPT does not work well, as becomes clear when one does a finite temperature study. At any finite  $T$ , while the IPT continues to show only one first order phase transition at which the AFM order turns on, the CTQMC shows, in addition, a second, continuous transition back to a PM phase, with its physics determined by the Heisenberg model. As  $T$  increases, the values of  $U$  corresponding to the first and the second order transitions approach each other, shrinking the  $U$  range for which the long range AFM order is stable. There is a line of tricritical point  $T_{\text{tcp}}$  that separates the two surfaces of first and second order phase transitions.

Recently the IHM has been realised in ultracold fermions by Esslinger's group on a 2-dimensional honeycomb lattice and it can be extended to higher dimensional layered honeycomb lattice by introducing perpendicular hopping. Though our numerical study is on the Bethe lattice of infinite connectivity, we expect the qualitative physics to be the same for any bipartite lattice in  $d \geq 2$  which has a compact density of states (DOS) like the DOS of the Bethe lattice of infinite connectivity. By choosing a large enough  $\Delta$ , it might be possible to realise an AFM phase for the IHM in experiments where the AFM order turns on with a first order transition and is lost by a second order transition by tuning  $U$ .

It would be interesting to look for signatures of the various effects we have discussed, including the quantum phase transition, in the experimental measurements in such systems.

This work is in collaboration with Soumen Bag (research scholar at Indian Institute of Sciences(IISc), Bangalore) and H. R. Krishnamurthy (IISc, Bangalore)}.

Reference: Phys. Rev. B **91**, 235108 (2015).

**6. Combined effect of disorder and e-e interactions in graphene:** We are currently studying combined effect of disorder and e-e interactions in graphene. For highly doped graphene, where the screening is good, charge impurities are expected to produce a short range (SR) impurity potential like in Anderson model. In this case, all the single particle states including the Dirac states get localized with any infinitesimal strength of disorder. We are trying to see effect of e-e interaction on this localized system and ask the question how interactions in this 2-dimensional system helps in delocalizing. Further, we also study the effect of e-e interactions in the presence of long range (LR) impurities (which we described in earlier section) in which the non-interacting system has shown indications of a single particle mobility edge. We have treated both disorder and e-e interactions exactly in the spinless model of fermions on honeycomb lattice with nearest neighbour interaction using exact diagonalization. We found that for the case of short range disorder, in the interacting system a dynamical transition occurs which is consistent with predictions from perturbative treatment of interactions by Basko et.al. For a given strength of interaction, there exist a many-body mobility edge which separates the localized many-body states from the extended states. Indication in support of the many-body ME are obtained from analysis of normalised participation ratio in Fock space and from the variance of the Renyi entropy. %Further we showed that even inside the many body localized regime, system obeys eigenstate thermalization hypothesis and the Renyi entropy follows volume law. But more interesting thing from the point of view of graphene is that For weak interactions though a larger sector of many-body states in the middle of the spectrum are delocalised by interactions, ground state and many of low energy excited states are still localized even in the presence of interactions. But for interaction strength  $V \sim 2t$  which is supposed to be a good estimate of e-e interactions in graphene, the entire many-body spectrum gets delocalised. In the case of LR impurities, where in the absence of interactions single particle states near the band center (Dirac states) are extended for weak disorder while states at the band edges are localized, interactions do not hybridise localized and extended states. Even in this case many-body spectrum

has mobility edges. Compared to the case of short range impurities, here comparatively a weaker strength of e-e interactions can delocalise all the many body states. \

This analysis not only answers important questions relevant in context of graphene, but also provide answer to very important question about stability of many-body localized phase in 2-dimensions. Recent work has shown that due to Griffith effects, MBL might not always be stable in a system of dimension more than one. Our numerical work provides an example of a system where MBL can survive in 2-dimensions.

This work is done in collaboration with my student Sabyasachi Nag (SINP).

Reference : Manuscript under preparation

## Dr. (Ms) Barnana Pal

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India.

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1. Date of birth : September 20, 1959.
2. Present position : Professor(F), Grade: Rs. 37400-67400/\_  
GP: Rs. 8700/\_
3. Academic qualifications : Ph. D. (University of Calcutta), 1992.  
Post M. Sc. (Saha Institute of  
Nuclear Physics), 1983.  
M. Sc. (University of Calcutta), 1st Class, 1981.  
B. Sc. (University of Calcutta), 1st Class, 1979.
4. Membership of professional bodies : Life member of the Acoustical Society of India,  
Ultrasonic Society of India and  
The Indian Physical Society.
5. Professional Career : Professor 'F' 01.08.2007 onwards  
Associate Professor 'E' 01.02.2003 - 31.07.2007  
Reader(SD), 01.02.1997 - 31.01.2003  
Lecturer(SC), 05.12.1992 - 31.01.1997  
Scientist(SB), 27.08.1990 - 05.12.1992  
SRF-2 (SINP) 19.11.1985 - 27.08.1990  
SRF-1 (SINP) 19.11.1983 - 18.11.1985

### 6. Research Interest

: Field of interest is Condensed Matter Physics.

Ultrasonic characterization of solids and liquids using pulse-echo, coherent pulse/cw and RUS techniques, "propagating wave" analysis of observed acoustic responses and development of Fourier acoustical methods.

Modeling and Monte-Carlo simulation on systems for the study of cluster formation, growth, stability and ordering, phase transitions in monolayer and other systems with competing interactions.

Green's Function theory, phonon-phonon interaction.

### 7. Participation in National/International Conferences/Symposia:

- i. *XXIst National Symposium on Ultrasonics*, held at S N Bose National Centre for Basic Sciences, Kolkata, during 08-10 November, 2016, Organized by S N Bose National Centre for Basic Sciences and Ultrasonics Society of India.  
Barnana Pal, **Co-Convener**.

- ii. Conference on “*New Advances in Acoustics (NAA 2015)*”, held at Sanghai, China, during Jan 31 to Feb 02, 2015. **Oral Presentation.**
- iii. Seminar on “*Economic Growth and National Integration*” organized by India International Friendship Society held at India International Centre, New Delhi on 26<sup>th</sup> March 2014, Invited participant.
- iv. One-Day Seminar under “DBT-STAR College Program” held at Lady Brabourne College, Kolkata on Dec 07, 2013, **Invited Lecture.**
- v. 1<sup>st</sup> International Conference on *Frontiers in Computational Physics: Modeling the Earth System*, 16-20 Dec, 2012, National Center for Atmospheric Research, Boulder, CO, USA, organized by ELSEVIER, **oral presentation.**
- vi. Young Physicists' Colloquium, YPC-2011 organized by Indian Physical Society, **Convener.**
- vii. “CSIR Programme on Youth for Leadership in Science”, Dec 31, 2009, held at Central Mechanical Engineering Research Institute, Durgapur, W B, India, **Invited Lecture.**
- viii. Discussion Meeting on Developing our Collective Vision for the future (Sub-topic: Condensed Matter Physics), Indira Gandhi Centre for Atomic Research, Kalpakkam, April 29-30, 2004, **poster presentation.**
- ix. National Symposium on Ultrasonics (XII-NSU), Guru Nanak Dev University, Amritsar, November 3-5, 2003, **oral presentation.**
- x. Condensed Matter Days 2003, Dept. of Physics, Jadavpur University, Kolkata, August 27-29, 2003, **contributed Paper.**
- xi. Conference on Strongly Correlated Electron Systems, SINP, Calcutta, October 23-28, 2000, **contributed paper.**
- xii. Symposium on Condensed Matter Physics, Indian Association for the Cultivation of Science, Calcutta, December 4-6, 1999, **contributed paper.**
- xiii. National Symposium on Acoustics, Indian Association for the Cultivation of Science, Calcutta, December 18-20, 1998, **oral presentation.**
- xiv. School on Complex Systems, Indian Association for the Cultivation of Science, Calcutta, January 30-February 3, 1995, **contributed paper.**
- xv. VI- National Symposium on Ultrasonics, Srivenkateswara University, Tirupati, September 16-17, 1994, **oral presentation.**
- xvi. National Symposium on Acoustics, IIT Madras, December 13-14, 1992, **oral presentation.**
- xvii. IV-National Symposium on Ultrasonics, National Physical Laboratory, New Delhi, September 21-22, 1989, **oral presentation.**
- xviii. Raman Centenary Year Symposium on Acoustics, IISc Bangalore, October 25-28, 1988, **oral presentation.**
- xix. Solid State Physics Symposium, Nagpur, December 27-30, 1985, **poster presentation.**

## 8. Special awards, honours or distinctions:

**Bharat Jyoti Award** awarded by India International Friendship Society on 26<sup>th</sup> March 2014 at India International Centre, New Delhi.

## 9. Teaching experience:

Teaching experience in Post M.Sc. (Physics) at SINP (Basic Course, Advanced Course, Advanced Experiments on Condensed Matter Physics) and in project Guidance for M.Sc. (Physics) Students under Summer Students' Programme.

### 10. Research planning, management, organizing and guiding experience:

- Conducting research and developmental work in the Ultrasonic Laboratory of SINP since 1983. Experimental facilities presently available are: Pulse-echo set-up, Resonant Ultrasound Spectrometer, Solution growth of single crystals, Vacuum coating unit with thickness monitor. Fourier Transform Pulse-echo is under investigation.
- Conducting Advanced Experiments on Condensed Matter Physics for Post M.Sc. course since 1993.
- Guiding project students under Summer Students' Programme since 2006.
- Convener of YPC-2011 organized by Indian Physical Society.
- Member of the local organizing committee for International Conference on Magnetic Materials (ICMM), Dec 11-16, 2007, organized by SINP.

## 11. List of publications :

Publications from 2007 onwards (Total 10 publications, 6 single author)

### Articles in peer reviewed International Journals:

1. "Fourier Transform Ultrasound Spectroscopy For the Determination of Wave Propagation Parameters", **Barnana Pal**, Ultrasonics 73 (2017) 140–143, doi:<http://dx.doi.org/10.1016/j.ultras.2016.09.008>, [arXiv:1605.04678v1](https://arxiv.org/abs/1605.04678v1)
2. "Condensation Under Controlled Cooling: A Simulation Study", **Barnana Pal**, International Journal of Emerging Technology and Advanced Engineering, 7 (2017) 92-96, [arXiv:1308.6655v1](https://arxiv.org/abs/1308.6655v1).
3. "Pulse-echo method cannot measure wave attenuation accurately", **Barnana Pal**, Ultrasonics 61 (2015) 6-9, <http://dx.doi.org/10.1016/j.ultras.2015.03.005>, [arXiv:1411.4374](https://arxiv.org/abs/1411.4374).
4. "Anomalous Ultrasonic Attenuation in Aqueous NaCl Solutions", **Barnana Pal** and Srinanda Kundu, Universal Journal of Chemistry 1(3) pp- 96-101, 2013 DOI: 10.13189/ujc.2013.010304, arXiv: 1206.2779v2. (Major part of this experiment and complete data analysis have been done by the first author. S Kundu helped in experiments and suggested a few important points in writing the manuscript)
5. "Ordering in Two-Dimensional Lennard-Jones Clusters", **Barnana Pal**, ISRN Condensed Matter Physics, 2012 (2012), Article ID 342642, 7 pages, doi:10.5402/2012/342642.
6. "Relaxation dynamics in small clusters: A modified Monte Carlo approach", **Barnana Pal**, Journal of Computational Physics, 227(2008) pp.2666-2673.

### Article in Conference Proceedings:

7. "Incidence of ultrasonic wave through Newtonian and non-Newtonian fluids", Md Sarowar Hossain\*, Animesh Basak\* , **Barnana Pal** and P K Mukhopadhyay\*, XXIst National Symposium on Ultrasonics, 08-10 November, 2016, Organized by S N Bose National Centre for Basic Sciences and Ultrasonics Society of India. (Experiment is done in the Ultrasonic Lab of SINP)  
(Best poster awarded by Ultrasonics Society of India)

8. "Development of pulse-echo technique to measure the ultrasonic properties", Dipanjan Samanta\*, Sarowar Hossain\*, **Barnana Pal** and P.K. Mukhopadhyay\* , Proceedings of Indian Workshop & Symposium on Modeling, Experimentation & Simulation on Complex Systems, MESCOs 2015, Aug 5-7, 2015, Organized by Haldia Institute of Technology, Haldia, WB, p-63.

\* S.N. Bose National Centre for Basic Sciences, Salt Lake, Kolkata-98, India

### Article in Book:

9. "Nonlinear Jeans instability in a uniformly rotating gas", Nikhil Chakrabarti, **Barnana Pal** and Vinod Krishan\*\*, *Turbulence, Dynamos, Accretion Discs, Pulsars and Collective Plasma Processes*, S. S. Hasan, R. T. Gangadgara and V. Krishan (eds.), Springer, 2008, p-281.

### Article in other Journals:

10. "Ultrasound for Medical Diagnostic and Therapeutic Application", **Barnana Pal**, J. Ananda Mohan College, **3**(2008)41 (Invited Article).

### Publications prior to 2007.

11. "Signature of glass transition in strongly correlated 2D liquid", Haimanti Chakrabarti<sup>1</sup> and **Barnana Pal**, Journal of Physics: Condensed Matter, **18**(2006) 9323.
12. "Distorted Waves for the Study of Dispersion", **Barnana Pal**, Santwana Raychaudhuri and Yoshinobu Kawai", Physics of Plasmas, **12**(2005)062306.
13. "Ultrasonic pulse propagation in a linear dispersive medium", **Barnana Pal** and Santwana Raychaudhuri, Journal of Pure and applied Ultrasonics, **26**(2004) 63.
14. "Diffusion in a strongly correlated 2-D liquid system", Haimanti Chakrabarti<sup>1</sup> and **Barnana Pal**, Indian Journal of Physics, **78**(9) (2004) 935.
15. "Acoustic attenuation in brass", **Barnana Pal**, Japanese Journal of Applied Physics, Pt-1, **42**(2003) 5813.
16. "Elastic stiffness properties of brass near the order-disorder transition - an overview", **Barnana Pal**, Japanese Journal of Applied Physics, Pt-1, **40** (2001) 5054.
17. "Elastic properties of beta-brass near its order-disorder transition – an overview", **Barnana Pal**, Journal of the Acoustical Society of India, **XXVI** (1998) 199.
18. "Response of a composite resonator under pulse excitation – a numerical study, **Barnana Pal**, Japanese Journal of Applied Physics Pt-1, **35** (1996) 4839.

19. "Diffusion in complex liquid surfaces – a Monte Carlo study, Haimanti Chakrabarti<sup>1</sup> and **Barnana Pal**, Indian Journal of Physics, **70A** (1996) 729.
20. "Ultrasonic study of beta-brass", **Barnana Pal**, Journal of Pure and Applied Ultrasonics, **17** (1995) 63.
21. "Monte Carlo simulation on a rigid-rod model for a Langmuir monolayer", **Barnana Pal**, Sujata Modok and Alokmay Datta, Surface Science, **310** (1994) 407.
22. "Response of a solid sample under acoustic excitation", **Barnana Pal**, Journal of the Acoustical Society of India, **XX(1-4)** (1992) 79.
23. "Ultrasound propagation in high- $T_c$  superconducting sample  $YBa_2Cu_{3.1}O_x$  (doped with ~10% Ag)", **Barnana Pal** and S K Sinha, Journal of Pure and applied Ultrasonics **13** (1991) 7.
24. "CW and pulse response of a mechanical resonator: Numerical evaluation and Experimental observations", **Barnana Pal** and S K Sinha, Japanese Journal of Applied Physics Pt-1, **29** (1990) 2837.
25. "Monte-Carlo phase diagram of an Ising system with isotropic competing interaction", **Barnana Pal** and Subinay Dasgupta, Zeitschrift fur Physik B-Condensed Matter, **78** (1990) 489.
26. "Response of a solid sample of finite length to the exciting electromagnetic pulses of very large, medium and very short duration", **Barnana Pal** and S K Sinha, Journal of the Acoustical Society of India, **XVI** (1988) 200.
27. "Structural instabilities of DLA- like fractals at finite temperatures", **B Pal**, S S Manna and B K Chakraborti, Solid State Communication, **64** (1987) 1309.

### Articles in Conference Proceedings:

28. "The long pulse technique reviewed on the basis of the propagating wave model", **Barnana Pal**, Proceedings of the Seventh National Symposium on Ultrasonics, September 6-7, (1996) 175.
29. "Simulation studies on a monolayer of rigid rod-like molecules", **Barnana Pal**, Sujata Modok and Alokmay Datta, Proceedings of the DAE Solid State Physics Symposium, **35C** (1992) 444.
30. "Transverse acoustic attenuation in crystals", S K Sinha and **B Pal**, Proceedings of the DAE Solid State Physics Symposium, **28C** (1985) 214.

(13 single author out of 30 publications)



## Highlights of works done since 2012:

### I. Pulse-echo method can't measure wave attenuation accurately

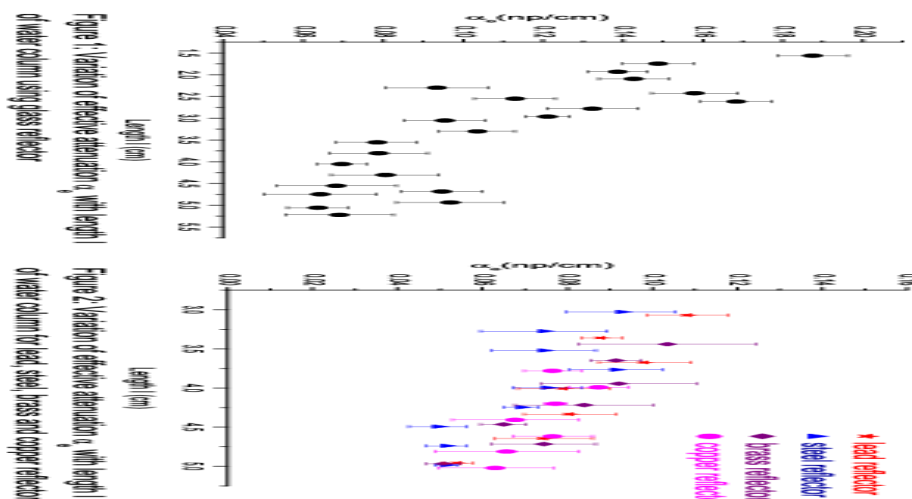
Various techniques have been devised for accurate measurement of acoustic wave attenuation  $\alpha$  in solids and liquids. Still, a wide variation is observed in the attenuation values in different materials reported in the literature. Present numerical study based on a 'propagating wave' model analysis clearly shows that the attenuation constant  $\alpha_e$  obtained from exponential fitting of the echo heights in pulse-echo method depends on sample length  $l$ , propagation constant  $k$  and wave reflection constant  $r$  at the boundary in a complicated manner. Accurate determination of  $\alpha$  is possible from the pulse-echo signal with the application of a Fourier transform computational method. This requires Fourier analysis of the echo-pattern obtained for several known sample lengths under similar experimental conditions so as to keep  $r$ ,  $k$  and  $\alpha$  constant. Knowing the amplitudes obtained for various sample lengths for a particular component wave, a computational method of parameter fitting may be adopted to find out accurate values for  $r$ ,  $k$  and  $\alpha$ .

**This work is important to solve a long-standing problem of accurate measurement of ultrasonic attenuation in solids & liquids and has been published in the peer reviewed international journal *Ultrasonics*, 61 (2015) 6-9.**

### II. Fourier transform ultrasound spectroscopy (FTUS) for the determination of wave propagation parameters

From the theoretical analysis based on propagating wave model, we have shown that the attenuation constant, obtained from pulse-echo method is an effective value ( $\alpha_e$ ), dependent on sample length ( $l$ ) and wave reflection constant ( $r$ ) at the sample boundary and is different from its actual or intrinsic value  $\alpha$ . This has been verified experimentally. Figures 1 and 2 show the results. Variation of  $r$  is done using different reflector materials, viz., steel, brass, copper, lead and glass having different mechanical impedances.

Based on the above observation, we propose Fourier Transform Ultrasound Spectroscopy (FTUS) to be an effective solution for determining more accurate values for the parameters  $\alpha$ ,  $r$  and  $k$ , the propagation constant. Pulse-echo signals obtained under same experimental conditions regarding the exciting input signal and reflecting property at the boundary for various sample lengths, are captured. The Fourier amplitudes of the component waves of these echo signals are computed and compared with theoretical values over the frequency range where the amplitudes are considerably high. This is done using Oak Ridge and Oxford method of parameter fitting. For



tri-distilled water at room temperature (25°C) at 1MHz frequency, we get  $\alpha = 0.0435 \pm 0.0013$  np/cm and  $k = 42.74 \pm 0.03$  cm<sup>-1</sup>. The results are summarized in Table-1. The parameters thus obtained are more accurate and consistent with the work reported by R. Martinez et al. [ref: R. Martinez, L. Leija, A. Vera, Ultrasonic attenuation in pure water: Comparison between through-transmission and pulse-echo techniques, [2010 Pan American Health Care Exchanges-PAHCE](http://dx.doi.org/10.1109/PAHCE.2010.5474593), 15-19 March 2010, IEEE, Lima, Peru, 81-84, <http://dx.doi.org/10.1109/PAHCE.2010.5474593>].

**Table-I: Input parameters and best fit output parameters**

Reflector material	Input parameters			Best fit output parameters				
	k (cm <sup>-1</sup> ) (experimental)	r (calculated)	$\alpha_e$ (np.cm <sup>-1</sup> )	k (cm <sup>-1</sup> )	Av k (cm <sup>-1</sup> )	r	$\alpha$ (np.cm <sup>-1</sup> )	Av $\alpha$ (np.cm <sup>-1</sup> )
Steel	42.72	0.94	0.0497	42.76	42.74±0.03	0.92	0.0439	0.0435±0.0013
Copper		0.93	0.0619	42.72		0.91	0.0422	
Brass		0.93	0.0510	42.77		0.91	0.0455	
Lead		0.89	0.0517	42.69		0.87	0.0418	
Glass		0.81	0.0639	42.76		0.80	0.0440	

Barnana Pal, Ultrasonics 73 (2017) 140–143, doi:<http://dx.doi.org/10.1016/j.ultras.2016.09.008>, [arXiv:1605.04678v1](https://arxiv.org/abs/1605.04678v1)

### III. Anomalous Ultrasonic Attenuation in Aqueous NaCl Solutions:

Aqueous electrolytes of various degrees of dilution show interesting features due to the complex character of the water molecules and their interaction with the anions and cations present in the solution. Formation of hydration shells in pure water, and ion-solvent clusters in aqueous electrolytic solutions have been evidenced in various experiments. The spatial extents of such hydration shells or ion-solvent clusters are not well understood. There is no well-defined structural model for these complex systems and more experimental study is needed. We have measured the ultrasonic velocity ( $v$ ) and attenuation constant ( $\alpha$ ) for wave frequencies 1MHz and 2MHz on aqueous sodium chloride solutions over the full concentration ( $c$ ) range, 0–5.3 mol·L<sup>-1</sup> (saturated) at room temperature (25° C). This is the first reported data on ultrasonic measurement covering the full concentration range. The velocity ( $v$ ) shows an overall increase with the increase of  $c$  indicating comparatively stronger bonding among the ions and water molecules in the solution. The velocity values are in good agreement with other reported values for lower solution concentration. The attenuation plots, besides showing an overall increase with  $c$ , show the presence of two distinct attenuation peaks both for 1MHz and 2MHz waves. The overall increase in the attenuation value may be understood from an analysis based on existing theoretical background. In explaining the attenuation peaks, if it is assumed that scattering from ion-solute clusters formed in the aqueous solution are responsible, the predicted size of such clusters comes out to be ~ 25 microns. This is sufficiently large in comparison to those evidenced in other experiments.

Barnana pal & Srinanda Kundu, UJC 1(3) pp- 96-101, 2013 DOI:10.13189/ujc.2013.010304, [arXiv:1206.2779v2](https://arxiv.org/abs/1206.2779v2)

### IV. Relaxation Dynamics in Lennard-Jones systems:

The transformation of matter from high temperature disordered state to an equilibrium one depends strongly on the external, e. g. pressure ( $P$ ) and temperature ( $T$ ), and internal physical condition, the interaction potential ( $V$ ) of the constituent atoms. The study of the relaxation dynamics of such systems is important for various practical applications. We use Monte-Carlo (MC) method to investigate the dynamics considering a realistic model in which the constituent particles of the system are free to move and take any

position in a two-dimensional space. The particles are assumed to be mono-atomic interacting through Lennard-Jones (L-J) potential. A modified Metropolis algorithm to incorporate real thermal motion is introduced. The important results are the following:

i. Cluster formation in a two-dimensional Lennard-Jones system under different conditions of temperature ( $T$ ) and particle concentration ( $c$ ) has been studied. The  $c$ - $T$  phase diagram determined from the study of the root mean square displacement of the particles in the equilibrium configuration shows features characteristics of the  $P$ - $T$  diagram for phase equilibrium in real systems. The solid-like to liquid-like transition takes place when the average nearest neighbour distance increases by  $\sim 1\%$  of the equilibrium value in the low-temperature solid-like configuration. The Lindemann parameter ( $\delta$ ) is found to decrease with the increase of  $c$  to reach a steady value of  $\delta = 0.0106 \pm 0.0004$  for  $c \geq 0.6$ .

Barnana Pal, ISRN Condensed Matter Physics, Volume 2012, Article ID 342642, 7 pages, doi:10.5402/2012/342642

ii. The formation, growth, structure and cluster size distribution (CSD) properties under annealing condition have been studied. The system, initially at relatively higher temperature  $T_i$ , undergoes temperature reduction following exponential law with decay constant  $\alpha$  to a lower temperature  $T_f$  and subsequently reaches equilibrium. The equilibrium phase configuration depends strongly on the number density  $c$  of particles and  $\alpha$ . The root mean square particle displacement in the final equilibrium phase shows maximum value for  $\alpha = \alpha_c \sim 10^{-3}$  for all  $c$ . The CSD properties obtained at  $\alpha = 10^{-3}$  shows a sharp peak in the lower cluster size region for low  $c$ . The peak shifts towards higher cluster size for lower  $\alpha$ . The CSD fits well with a modified Gamma distribution function. All of the particles in the system form a single cluster when  $c$  is larger than a critical value  $c_c$  ( $\sim 0.5$ ). A compact well-defined ordered structure is obtained for  $c \geq c_c$  and  $\alpha \ll \alpha_c$ .

**Barnana Pal**, International Journal of Emerging Technology and Advanced Engineering, 7 (2017) 92-96, [arXiv:1308.6655v1](https://arxiv.org/abs/1308.6655v1).

## V. Developmental Work

**Resonant Ultrasound Spectrometer – New facility:** Resonant ultrasound spectroscopy is an efficient method for the determination of the elastic constant matrix for single crystals of relatively small size ( $\sim 1 \text{ mm}^3$ ) in the form of a parallelepiped or a cylinder with high accuracy and from a single measurement. The spectrometer (RUSpec) from M/S Hesselmann& Kohler, Germany has been procured and installed in the ultrasonic laboratory. It is a new facility for the study of various samples of present day interest.

## **Prof. Bikas K. Chakrabarti**

**1. Present Staff:** Sr. Professor I

**2. Ph. D. Students since 2012:**

A. Ghosh (2014), Post Doc. In Aalto Univ. of Technology, Helsinki;

S. Biswas (2015), Post Doc. at Max Planck Inst , Goettingen;

A. Rajak (Jointly with A. Basu; 2016), Post Doc. at Bar Ilan Univ., Ramat Gan.

**3. Important equipment & facility:** NA

**4. Research highlight (Since 2012):** Researches in Quantum Annealing & Econophysics.

### **Books & their citations from Google Scholar:**

**Quantum Spin Glasses, Annealing and Computation,** BK Chakrabarti, J Inoue, R Tamura, S Tanaka, Cambridge University Press (2017)  
(Citation: 01)

**Quantum Phase Transitions in Transverse Field Spin Models,** A Dutta, G Aeppli, BK Chakrabarti, U Divakaran, TF Rosenbaum, D Sen, Cambridge University Press (2015)  
(Citation: 128)

**Statistical Physics of Fracture, Beakdown, and Earthquake: Effects of Disorder and Heterogeneity,** S Biswas, P. Ray, BK Chakrabarti, Wiley (2015)  
(Citation: 12)

**Econophysics of income and wealth distributions,** BK Chakrabarti, A Chakraborti, SR Chakravarty, A Chatterjee, Cambridge University Press (2013)  
(Citation: 106)

**Sociophysics: an introduction,** P Sen, BK Chakrabarti, Oxford University Press (2013)  
(Citation: 119)

**Quantum Ising phases and transitions in transverse Ising models,** S Suzuki, J Inoue, BK Chakrabarti, Springer (2012)  
(Citation: 408)

## Papers & their citations from Google Scholar:

**Fat tailed distributions for deaths in conflicts and disasters**, A Chatterjee, BK Chakrabarti, Reports in Advances of Physical Sciences **1** (01), 1740007 (2017)  
(Citation: 02)

**Socio-economic inequality: Relationship between Gini and Kolkata indices**, A Chatterjee, A Ghosh, BK Chakrabarti, Physica A: Statistical Mechanics and its Applications **466**, 583-595 (2017)  
(Citation: 01)

**Inequality measures in kinetic exchange models of wealth distributions**  
A Ghosh, A Chatterjee, J Inoue, BK Chakrabarti,  
Physica A: Statistical Mechanics and its Applications **451**, 465-474 (2016)  
(Citation: 03)

**Can economics afford not to become natural science?** BK Chakrabarti,  
European Physical Journal Spl. Topics **225**, 3121-3125 (2016)  
(Citation: 00)

**Universality of citation distributions for academic institutions and journals**,  
A Chatterjee, A Ghosh, BK Chakrabarti, PloS one **11** (1), e0146762 (2016)  
(Citation: 15)

**Classical-to-quantum crossover in the critical behavior of the transverse-field Sherrington-Kirkpatrick spin glass model**, S Mukherjee, A Rajak, BK Chakrabarti,  
Physical Review E **92** (4), 042107 (2015)  
(Citation: 02)

**Measuring social inequality with quantitative methodology: analytical estimates and empirical data analysis by gini and k indices**, J Inoue, A Ghosh, A Chatterjee, BK Chakrabarti, Physica A: Statistical Mechanics and its Applications **429**, 184-204 (2015)  
(Citation: 19)

**Statistical mechanics of competitive resource allocation using agent-based models**,  
A Chakraborti, D Challet, A Chatterjee, M Marsili, YC Zhang, BK Chakrabarti,  
Physics Reports **552**, 1-25 (2015)  
(Citation: 45)

**Social inequality: from data to statistical physics modeling**, A Chatterjee, A Ghosh, J Inoue, BK Chakrabarti, Journal of Physics: Conference Series **638** (1), 012014 (2014)  
(Citation: 02)

**Zipf's law in city size from a resource utilization model**, A Ghosh, A Chatterjee, AS Chakrabarti, BK Chakrabarti, Physical Review E **90** (4), 042815 (2014)  
(Citation: 05)

**Inequality in societies, academic institutions and science journals: Gini and k-indices**, A Ghosh, N Chattopadhyay, BK Chakrabarti, Physica A: Statistical Mechanics and its Applications **410**, 30-34 (2014)  
(Citation: 23)

**Multivariable optimization: Quantum annealing & computation**, S Mukherjee, BK Chakrabarti, European Physical Journal **224**, 17-24 (2014)  
(Citation: 12)

**Response of the two-dimensional kinetic Ising model under a stochastic field**, A Ghosh, BK Chakrabarti, Journal of Statistical Mechanics: Theory and Experiment **2013** (11), P11015 (2013)  
(Citation: 01)

**Self-organized dynamics in local load-sharing fiber bundle models**, S Biswas, BK Chakrabarti, Physical Review E **88** (4), 042112 (2013)  
(Citation: 03)

**Crossover behaviors in one and two dimensional heterogeneous load sharing fiber bundle models**, S Biswas, BK Chakrabarti, European Physical Journal B **86**, 160 (2013)  
(Citation: 06)

**Statistical physics of fracture, friction, and earthquakes**, H Kawamura, T Hatano, N Kato, S Biswas, BK Chakrabarti, Reviews of Modern Physics **84** (2), 839 (2013)  
(Citation: 78)

## **5. Brief CV: Presently Editorial Board Member of:**

### **JOURNALS:**

- a) European Physical Journal B (Executive Editor)
- b) Indian Journal of Physics
- c) Journal of Economic Interaction and Coordination
- d) Journal of Magnetism and Magnetic Materials
- e) Scientific Reports
- f) SciPost

### **& BOOK SERIES:**

- a) Physics of Society: Econophysics & Sociophysics (with M. Gallegati, A. Kirman & H. E. Stanley) of Cambridge University Press; b) Statistical Physics of Fracture & Breakdown (with Purusattam Ray), Wiley.

## Bilwadal Bandyopadhyay

**Topic: Preparation, characterization and study of magnetic properties of  $\text{Co}_x\text{Cu}_{1-x}$  ( $x = 0.01-0.7$ ) granular alloys**

Magnetic studies have been performed to characterize  $\text{Co}_{0.3}\text{Cu}_{0.7}$  granular alloy synthesized by chemical reduction. The alloy consists of superparamagnetic (SPM) particles with a mean size of 14 nm and a blocking temperature distribution extending to  $\sim 380$  K. Even at 4 K where the alloy is largely ferromagnetic, the average magnetic moment of cobalt is smaller than its expected value indicating that not all Co atoms contribute to ferromagnetism. Also, there exists an exchange bias field over a wide temperature range. These observations suggest that the particles have a Co rich SPM core, but outside the core region there is antiferromagnetic interaction between Co moments. The system has shown strong magnetic 'memory effect' which has been studied with various experimental protocols. The memory effect persists even at room temperature which could be technologically very interesting.

*Susmita Dhara, Rejeswari Roychowdhury and B. Bandyopadhyay*

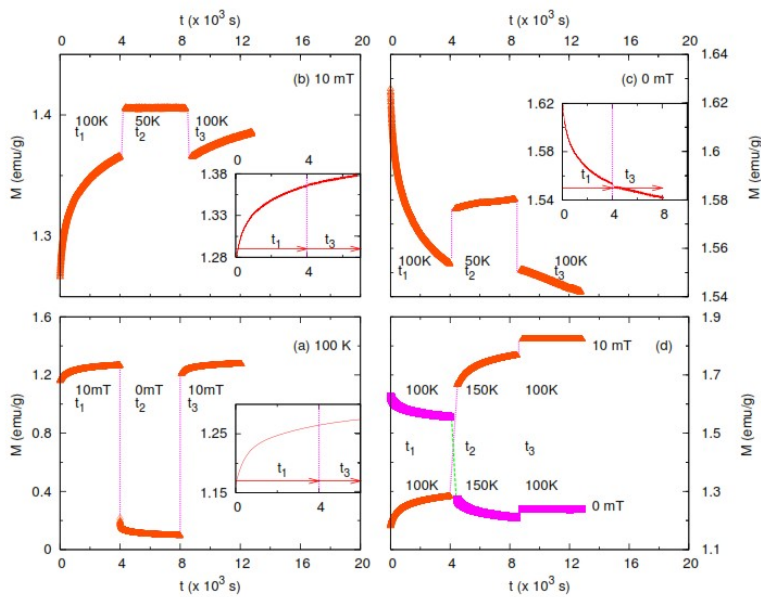


FIG. 8. (a) Magnetic relaxation at 100 K and 10 mT for  $t_1$  and  $t_3$  after cooling in ZFC mode with an intermediate measurement in zero-field for  $t_2$ . Inset shows the relaxation in 10 mT only. (b) Relaxation at 100 K and 10 mT for  $t_1$  and  $t_3$  after ZFC with an intermediate cooling at 50 K for  $t_2$ . Inset shows the relaxation at 100 K only. (c) Relaxation at 100 K at 0 mT for  $t_1$  and  $t_3$  after FC in 10 mT with an intermediate cooling at 50 K for  $t_2$ . Inset shows the relaxation at 100 K only. (d) Magnetic relaxation in zero and 10 mT after cooling in FC and ZFC modes, respectively, with an intermediate heating at 150 K.

**Topic: Effect of substitution at the transition metal site on the magnetic properties of rare earth ternary silicides**

In intermetallic compounds  $RE\text{Co}_2\text{Si}_2$  (Re = Pr and Nd), cobalt has been partially substituted by vanadium to obtain  $RE(\text{Co}_{1-x}\text{V}_x)_2\text{Si}_2$  ( $0 \leq x \leq 0.35$ ). The present study demonstrates that in these compounds where 3d and 4f ions occupy different layers in the crystal structure, V substitution and subsequent lattice expansion results in the occurrence of inequivalent magnetic ions and complex interactions that lead to multiple magnetic transitions. At temperatures around 40-50 K, the temperature dependence of magnetization indicates a ferrimagnetic transition which is accompanied by a rapid decrease in the temperature dependence of resistivity. Below temperatures  $\sim 30$  K, the samples begin to



show ferromagnetic-like behavior with the appearance of a coercive field and saturation in the magnetization at magnetic fields above  $\sim 2$  T. These two magnetic transitions are indicated also by prominent  $\lambda$ -like peaks in specific heat measurements. At around 10 K, a sharp drop in the resistivity indicates another magnetic transition which is followed by a rapid increase in coercive field with decrease in temperature. The onset of ferromagnetism at  $\sim 30$  K is accompanied with an exchange bias field which is observed for the first time in layered intermetallic compounds.

Rajeswari Roychowdhury, Susmita Dhara, and B. Bandyopadhyay

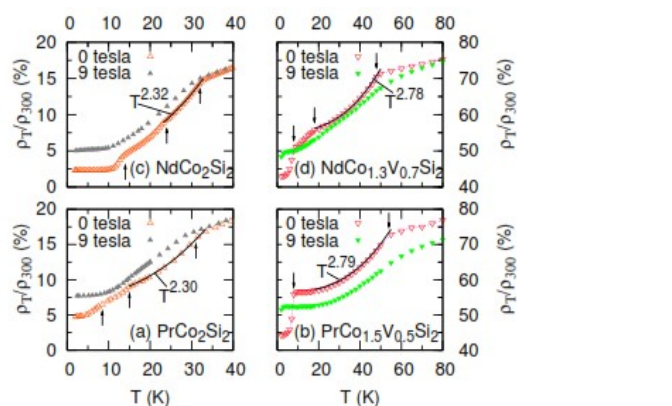


FIG. 7. Plots of resistivity  $\rho_T/\rho_{300}$  versus temperature in conditions of zero external magnetic field and in the magnetic field of 9 T for (a)  $\text{PrCo}_2\text{Si}_2$ , (b)  $\text{Pr}(\text{Co}_{0.75}\text{V}_{0.25})_2\text{Si}_2$ , (c)  $\text{NdCo}_2\text{Si}_2$ , and (d)  $\text{Nd}(\text{Co}_{0.65}\text{V}_{0.35})_2\text{Si}_2$ . The arrows show positions of phase transitions as reflected in zero field resistivity data, which, in (b) and (d) are joined by broken lines as a guide to the eye. The continuous lines joining some of zero-field data points are fit to the equation  $\rho_T/\rho_{300} = A + B T^\alpha$  with  $T^\alpha$  indicated in figures.

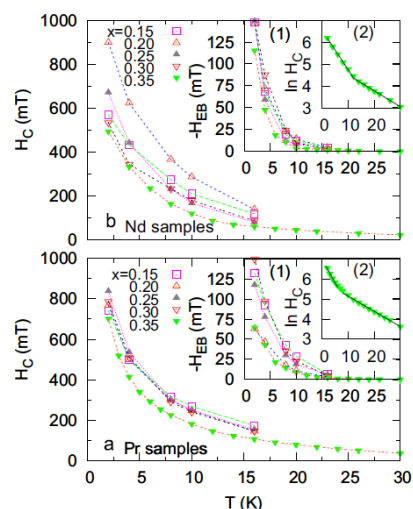


Fig. 7. (a) Temperature dependence of coercive field ( $H_C$ ) in (a)  $\text{Pr}(\text{Co}_{1-x}\text{V}_x)_2\text{Si}_2$  ( $x=0.15, 0.20, 0.25, 0.30$  and  $0.35$ ), and (b)  $\text{Nd}(\text{Co}_{1-x}\text{V}_x)_2\text{Si}_2$  ( $x=0.15, 0.20, 0.25, 0.30$  and  $0.35$ ). Inset (1): temperature dependence of exchange bias field ( $H_{EB}$ ) for the same samples. Inset (2): for  $\text{Pr,Nd}(\text{Co}_{0.65}\text{V}_{0.35})_2\text{Si}_2$  the plot of  $\ln H_C$  vs. temperature having two linear segments. The lines are guide to the eye.

### Topic: $\gamma$ -Radiation Induced Magnetic Modification and Iodide Sensing Property of Ag-Polyphenol Nanocomposite

Bio-synthesized silver polyphenol nanocomposite prepared by reducing  $\text{AgNO}_3$  with an aqueous extract of peanut skin, were characterized by TEM, XRD, UV-Vis absorption spectra, IR and magnetic measurements. Effect of low dose  $\gamma$  irradiation during the synthesis was studied and their physico-chemical properties were compared with those produced without irradiation. On the contrary to the diamagnetic behavior of bulk silver, the silver polyphenol nanocomposite thus prepared shows a significant ferromagnetic moment component. Exposure to  $\gamma$ -irradiation results in an exponential decay of ferromagnetic component.

Zarina Ansari<sup>1</sup>, Susmita Dhara, Bilwadal Bandyopadhyay, Abhijit Saha<sup>2</sup> and Kamalika Sen<sup>1</sup>

### Publications (2014 - ):

1. Synthesis, characterization and magnetic properties of  $\text{Co}_x\text{Cu}_{1-x}$  ( $x \sim 0.01-0.3$ ) granular alloys; S. Dhara, R. Roy Chowdhury, S. Lahiri, P. Ray and B. Bandyopadhyay, J. Magn. Magn. Mat. **374** (2015) 647–654.
2. Strong memory effect at room temperature in nanostructured granular alloy  $\text{Co}_{0.3}\text{Cu}_{0.7}$ ; S. Dhara, R. Roy Chowdhury and B. Bandyopadhyay, RSC Adv. **5** (2015) 95695-95702.

- Effect of vanadium substitution of cobalt in NdCo<sub>2</sub>Si<sub>2</sub>; R. Roy Chowdhury, S. Dhara and B. Bandyopadhyay, *Acta Physica Polonica* **A128** (2015) 530-532.
- Evidence of formation of Co<sub>x</sub>Cu<sub>1-x</sub> Nanoparticles with core-shell structure; S. Dhara, R. Roy Chowdhury and B. Bandyopadhyay, *Acta Physica Polonica* **A128** (2015) 533-535.
- Evidence of ferromagnetism in vanadium substituted layered intermetallic compounds RE(Co<sub>1-x</sub>V<sub>x</sub>)<sub>2</sub>Si<sub>2</sub> (RE = Pr and Nd;  $x \leq 0 \leq 0.35$ ); R. Roy Chowdhury, S. Dhara and B. Bandyopadhyay, *J. Magn. Magn. Mat.* **401** (2016) 998-1005.
- Spectral anion sensing and  $\gamma$ -radiation induced magnetic modifications of polyphenol generated Ag-nanoparticles, Z. Ansari <sup>a</sup>, S. Dhara, B. Bandyopadhyay, A. Saha <sup>b</sup> and K. Sen <sup>a</sup>, *Spectrochimica Acta* **A156** (2016) 98-104.
- Observation of resistivity minimum at low temperature in Co<sub>x</sub>Cu<sub>1-x</sub> ( $x \sim 0.17-0.76$ ) nanostructured granular alloys, S. Dhara, R. Roy Chowdhury, and B. Bandyopadhyay, *Phys. Rev. B* **93** (2016) 214413.

### Conference proceedings:

- Magnetization Study of Co<sub>x</sub>Cu<sub>1-x</sub> Nanoparticles; Susmita Dhara, Rajeswari Roy Chowdhury and Bilwadal Bandyopadhyay, *Phys. Procedia* **54** (2014) 38-44.
- Kondo Effect in Co<sub>x</sub>Cu<sub>1-x</sub> Granular Alloys Prepared by Chemical Reduction Method; Susmita Dhara, Rajeswari Roy Chowdhury and Bilwadal Bandyopadhyay, *AIP Conf. Proc.* **1665**, 130056 (2015); doi:10.1063/1.4918204.
- Ferromagnetism in Nd(Co<sub>1-x</sub>V<sub>x</sub>)<sub>2</sub>Si<sub>2</sub> ( $0 \leq x \leq 0.5$ ); R. Roy Chowdhury, S. Dhara and B. Bandyopadhyay, *Phys. Procedia* **54** (2014) 113 - 117.
- Crossover from Antiferro-To-Ferromagnetism on Substitution of Co by V in RE(Co<sub>1-x</sub>V<sub>x</sub>)<sub>2</sub>Si<sub>2</sub> ( $0 \leq x \leq 0.35$ ); Rajeswari Roy Chowdhury, Susmita Dhara and Bilwadal Bandyopadhyay, *AIP Conf. Proc.* **1665**, 130040 (2015); doi: 10.1063/1.4918188.

### Students:

Susmita Dhara, Title of thesis: Preparation, Characterization and Study of Magnetic Properties of Co<sub>x</sub>Cu<sub>1-x</sub> ( $0.01 \leq x \leq 0.7$ ) Granular Alloys, thesis submitted: May 2016; Ph.D. awarded: March 2017; Present position: post-doc fellow at IIT Bombay

Rajeswari Roychowdhury, Title of thesis: Effect of substitution at the transition metal site on the magnetic properties of rare earth ternary silicides, thesis submitted: October 2016

### Facilities:

Solid state NMR spectroscopy  
Liquid nitrogen and liquid helium production  
Magnetometer SQUID-vsm

<sup>a</sup>Department of Chemistry, University of Calcutta, 92, APC Road, Kolkata, India

<sup>b</sup>UGC-DAE Consortium for Scientific Research, Kolkata Centre, III/LB-8, Bidhananagar, Kolkata.

# Biswajit Karmakar

## Personal profile:

Date of birth: 5th June 1972  
Place of birth: North 24 Paraganas, West Bengal, India.  
Citizenship: Indian

## Contact Information:

Office: Saha Institute of Nuclear Physics. 1/AF Salt Lake, Kolkata-64, India.  
Phone: +91 3323370571 Ext-2464, Fax: +91 3323374637  
Email: biswajit.karmakar@saha.ac.in,  
biswajitkarmakar@gmail.com

## Educational Profile:

Present Position  
Associate Professor  
August, 2013  
Saha Institute of Nuclear Physics  
Kolkata, India

### Academic History

Researcher Scientist  
March, 2009-May, 2013  
NEST CNR and Scuola  
Normale Superiore. Pisa. Italy.

Postdoctoral Fellow  
March, 2006-December, 2008  
NEST CNR and Scuola  
Normale Superiore. Pisa. Italy.

Ph.D. in Physics  
22<sup>nd</sup> December 2005  
Tata Institute of Fundamental  
Research. Mumbai. India.

## Research Interests:

My research interests are optical spectroscopy and electronic transport study of semiconductor nanostructures and quantum Hall systems at dilution fridge temperatures under a high magnetic field. Using these studies I explore the correlated states of the semiconductor quantum structures and their physical properties. These studies of quantum physics will have direct implication in quantum information processing.

## Teaching Experience:

Since joining SINP in 2013, every year I teach Advanced Condensed Matter course to the post MSc students.

One student is doing Ph.D. on mesoscopic transport under my supervision at SINP.

## Invited Talks:

- **Experiments on quantum electron optics using quantum Hall edge states.** 59<sup>th</sup> DAE Solid State Physics Symposium, 2014, VIT University, Vellore, India.

- **Quantum simulations with artificial semiconductor lattice.** Meeting on Quantum Simulations, 2013, IISc. Bangalore, India.

## Journal papers:

- 1) **Quantum Hall realization of polarized intensity interferometry** by Krishanu Roychowdhury, Disha Wadhawan, Poonam Mehta, Biswajit Karmakar and Sourin Das. *Phy. Rev. B* **93** 220101(R) (2016).
- 2) **Nanoscale Mach-Zehnder interferometer with spin-resolved quantum Hall edge states** by Biswajit Karmakar, Davide Venturelli, Luca Chirolli, Vittorio Giovannetti, Rosario Fazio, Stefano Roddaro, Loren N Pfeiffer, Ken W West, Fabio Taddei and Vittorio Pellegrini. *Phy. Rev. B* **92** 195303 (2015).
- 3) **Anomalous low-temperature Coulomb drag in graphene-GaAs hetero-structures** by A Gamucci, D Spirito, M Carrega, B Karmakar, A Lombardo, M Bruna, LN Pfeiffer, KW West, AC Ferrari, Marco Polini and V Pellegrini. *Nature communications* **5** 5824 (2014).
- 4) **Magnetic catechin–dextran conjugate as targeted therapeutic for pancreatic tumour cells** by Orazio Vittorio, Valerio Voliani, Paolo Faraci, Biswajit Karmakar, Francesca Iemma, Silke Hampel, Maria Kavallaris and Giuseppe Cirillo. *Journal of Drug Targeting* **22** 408 (2014).

## Ph.D. Student:

Mr. Tanmay Maity (currently working on post MSc projects)

## Important equipment and facility:

Central Device Fabrication Facility consisting micro-fabrication with photolithography is set up. For cryogenic measurement up to 8 mK Temperature, a Dilution Refrigerator with superconducting magnet and optical windows is ordered and it is expected to install at the end of this year.

## Research highlights:

### 1. Targeted drug delivery:

Recently Catechin–dextran conjugates have attracted a lot of attention due to their anticancer activity against a range of cancer cells. Magnetic nano-particles have the ability to concentrate therapeutically important drugs due to their magnetic-spatial control by the external magnetic field and provide opportunities for targeted drug delivery for anticancer activity. For that reason we have modified the coating shell of commercial magnetic nanoparticles (Endorem) composed of dextran with the catechin–dextran conjugate. In our experiments, pancreatic tumor cells are grown on a Petri dish and the drug is added on the Petri dish after placing the dish on a permanent magnet. The magnetic field gradient attracts the nanomagnetic drug particles towards the magnet. As the Catechin–dextran conjugated with Endorem (Endo–Cat) is increased at the intracellular concentration of the drug and it induces apoptosis in 98% of pancreatic tumor cells placed under magnetic field. The conjugation of catechin–dextran with Endorem enhances the anticancer activity of this drug and provides a new strategy for targeted drug delivery on tumor cells driven by magnetic field. The ability to spatially control the delivery of the catechin–dextran by magnetic field makes it a promising agent for further application in cancer therapy.

## 2. Graphene-2DEG hybrid system:

There are current trends of research on hybrid systems which are composed of two different layers of materials. We have explored a heterostructure comprising a single-layer (or bilayer) graphene placed on a quantum well created in GaAs 31.5 nm below the top surface. Naturally the graphene is hole doped with characteristic linear dispersion (Dirac Fermions) and a high-mobility two-dimensional electron gas is composed of Schrodinger electrons. These are a new class of double-layer devices, composed of spatially-separated electron and hole fluids, with strong interlayer coulomb interaction. In this system we have performed coulomb drag experiments where a DC current is driven through one layer and the induced drag voltage is measured in the other layer. We find that the Coulomb drag resistivity significantly increases with decreasing temperatures below 5-10 K, following a logarithmic law. The low temperature logarithmic behavior displaying a notable departure from the ordinary  $T^2$  temperature dependence expected in a weakly-correlated Fermi liquid. This anomalous behavior is a signature of the onset of strong inter-layer correlations indicating formation of a condensate of excitons at zero magnetic field.

## 3. Quantum electron optics:

Quantum Hall system is the first example of a topological insulator, where the bulk gap is created by the application of a high perpendicular magnetic field. The topologically protected coherent edge states are useful for quantum information processing, where the edge states carry the quantum information and quantum interference effect performs flying qubit operation. Recently, a beam splitter, which prepares any superposition of the two logic states, is experimentally demonstrated by triggering a resonant charge transfer between spin resolved edge states (SRESs) at filling factor  $\nu = 2$  (number of field Landau level) by periodic in-plane magnetic field of the nano-magnet array placed at the boundary of the 2DEG. We fabricated a quantum interference device composed of a gate that introduces Aharonov-Bohm loop between the two nano-magnetic beam splitters. We have realized the quantum interference effect by tuning the Aharonov-Bohm flux. Experimental result shows visibility of quantum interference 12% at 250 mK and visibility decreases with increasing sample temperature. The observation of quantum interference effect in our device proves the coherency of charge transfer at the nano-magnetic beam splitters.

With this observation of quantum interference effect in spin resolved quantum Hall system, we have proposed theoretically two photon interferometer comprise of two set of source and four set of detectors. We have predicted entanglement in cross correlated noise between the two set of detectors with opposite spins.

## Future plan:

I want to focus in the direction of semiconductor nano-science research. In the clean nanostructure system I will explore quantum physics in view of implications in quantum information processing, quantum simulator, dynamics in quantum many body system etc. I will focus on the enhancement of visibility of quantum interference effect, study of cross-correlation in quantum point contact, realization of artificial quantum dot lattice and study of correlation in hybrid systems etc. For this reason, I have set up a central device fabrication facility. For experiment I am setting up an ultra-low temperature magneto-transport measurement facility. Apart from that to full fill my scientific program, I must need nanofabrication facility with electron beam lithography and other device processing systems which will be integrated in central device fabrication facility.

## Chandan Mazumdar

*Present position* : Professor-G  
*Division* : Condensed Matter Physics

### *Invited talks in conferences etc.*

- i) Griffiths phase in a frustrated antiferromagnetic intermetallic compound  $GdFe_{0.17}Sn_2$ , “International Conference on Magnetic Materials and Applications (ICMagMA - 2017)”, Defence Metallurgical Research Laboratory (DMRL), Hyderabad and Magnetism Society of India (MSI), 1-3 February, 2017 (Invited speaker).
- ii) Griffiths phase in a frustrated antiferromagnetic intermetallic compound  $GdFe_{0.17}Sn_2$ , “International Conference on Physics - 2016” Bangladesh Physical Society, Bangladesh and Atomic Energy Centre, Dhaka, Bangladesh, 10-12 March, 2016 (Invited speaker).
- iii) Antiferromagnetic ordering of  $Er_2NiSi_3$  compound, “International conference on Magnetic Materials and Applications (ICMagMA-2014)” Pondicherry University, Pondicherry, India, Sept. 15-17, 2014, (Invited speaker).
- iv) Inspirational talk on 24 Dec., 2013 in the INSPIRE internship science camp at Mahatma Gandhi Shikhsak Prashikshan Mahavidhyalaya, Banka, Bihar, with support of the DST, Ministry of Science & Technology, Government of India (22-26 Dec. 2013) (Mentor).
- v) Basic crystallography: Part-1 (Crystal system and Bravais Lattice) and Part II: Powder X-ray diffraction data analysis (methodology and examples), 1 July, 2013, 1<sup>st</sup> RC Material Science, Academic Staff College, Golapbag campus of the University of Burdwan, India, (28 June to 18 July, 2013) (Resource person).
- vi) Finding the CEF levels of f-electron systems using inelastic neutron spectroscopic studies (Case study:  $PrNi_2B_2C$ ), National Workshop on “Electron Dynamics in Magnetic Materials (EDMM-2013)”, DRDO complex, Chandipur, Odisha, 17-19 January 2013 (Invited speaker).

### *No. of Ph.D students*

#### From SINP:

- ☛ Mr. Santanu Pakhira (Thesis submitted in June'17)
- ☞ Ms. Sudipta Mondal (Thesis to be submitted by October'17)
- ☞ Miss. Binita Mondal (Work to be completed by March'18)
- ☛ Miss. Mily Kundu (Work to be completed by March'18)

#### External Student:

- ☛ Mr. Shovan Dan (jointly supervising with Dr. S. Mukherjee, Dept. of Physics, University of Burdwan)
- ☞ Ms. Sanchayita Mondal (Ex-SINP student, presently a lecturer in a local college)
- ☞ Supervised the experimental work of Mr. Krishanu Ghosh whose joint Ph.D thesis guides were Prof. R. Ranganathan (SINP) and Dr. S. Mukherjee, (Dept. of Physics, University of Burdwan) (Thesis submitted May'17)

## LIST OF PUBLICATIONS (2012-Contd.)

### *Papers published in International Journals*

- 1) Structural transformation in inverse-perovskite  $REPt_3B$  ( $RE = Sm, Gd-Tm$ ) associated with large volume reduction, Sudipta Mondal, Chandan Mazumdar, Rajarao Ranganathan and Maxim Avdeev, *Inorganic Chemistry*, (2017) (accepted for publication) (Impact factor: 4.820).
- 2) Magnetic frustration induced large magnetocaloric effect in the absence of long range magnetic order, Santanu Pakhira, Chandan Mazumdar, R. Ranganathan and Maxim Avdeev, *Scientific Reports*, (2017) (accepted for publication) (Impact factor: 5.228).
- 3) Role of the stability of charge ordering in exchange bias effect in doped manganites, Papri Dasgupta, Kalipada Das, Santanu Pakhira, Chandan Mazumdar, Sudip Mukherjee, S. Mukherjee and Asok. Poddar, *Scientific Reports*, **7** (2017) Article No. 3220 (Impact factor: 5.228).
- 4) Multiple crossovers between positive and negative magnetoresistance versus field due to fragile spin structure in metallic  $GdPd_3$ , Abhishek Pandey, Chandan Mazumdar, R. Ranganathan and D. C. Johnston, *Scientific Reports*, **7** (2017) Article No. 42789 (Impact factor: 5.228).
- 5) Large magnetic cooling power involving frustrated antiferromagnetic spin-glass state in  $R_2NiSi_3$  ( $R = Gd, Er$ ), Santanu Pakhira, Chandan Mazumdar, R. Ranganathan, S. Giri, and Maxim Avdeev, *Phys. Rev B*, **94** (2017) 104414 (Impact factor: 3.718 ; Times cited: 1).
- 6) Doping of Ga in antiferromagnetic semiconductor  $\alpha-Cr_2O_3$  and its effects on magnetic and electronic properties, R.N. Bhowmik, K. Venkata Siva, R. Ranganathan, Chandan Mazumdar, *Journal of Magnetism and Magnetic Materials*, **432** (2017) 56 (Impact factor: 2.357).
- 7) Zero thermal expansion with high Curie temperature in  $Ho_2Fe_{16}Cr$  alloy, Shovan Dan, S. Mukherjee, Chandan Mazumdar and R. Ranganathan, *RSC Adv.*, **6** (2016) 94809 (Impact factor: 3.289).
- 8) Absence of low energy magnetic spin-fluctuations in isovalently and aliovalently doped  $LaCo_2B_2$  superconducting compounds, M. Majumder, A. Ghoshray, P. Khuntia, C. Mazumdar, A. Poddar, M. Baenitz and K. Ghoshray, *Journal of Physics: Condensed Matter*, **28** (2016) 345701 (Impact factor: 2.209).
- 9) Griffiths phase behaviour in a frustrated antiferromagnetic intermetallic compound, Krishanu Ghosh, Chandan Mazumdar, R. Ranganathan and S. Mukherjee, *Scientific Reports*, **5** (2015) Article No. 15801 (Impact factor: 5.228 ; Times cited: 4).
- 10) Quaternary borocarbides: Relatively high  $T_c$  intermetallic superconductors and magnetic superconductors, Chandan Mazumdar and R. Nagarajan, *Physica C (Invited contribution to Special Issue on Superconducting Materials, dedicated to Theodore H. Geballe on the year of his 95<sup>th</sup> birthday)*, **514** (2015) 173 (Impact factor: 0.835 ; Times cited: 5).
- 11) Temperature dependence of resistivity of  $RFeAsO$  compounds, S. Mukherjee, Papri Dasgupta, Asok Poddar, and Chandan Mazumdar, *J. Theor. Appl. Phys.*, (2015) DOI 10.1007/s40094-015-0203-7 (7 pages).

- 12) Enhanced dielectric response of  $Gd_2Ti_2O_7$  nanoparticles in  $SiO_2$  matrix, Papri Dasgupta, S. Mukherjee, R.N. Bhowmik, Asok Poddar, Chandan Mazumdar, and R. Ranganathan, *Mater. Res. Bull.*, **50** (2014) 26 (Impact factor: 2.435). (Total Authors: 6 ; No. of Authors from SINP: 4)
- 13) On the evaluation of specific heat from thermoelectric power, Papri Dasgupta, Asok Poddar and Chandan Mazumdar, *Phys. Status Solidi B* **251** (2014) 877 (Impact factor: 1.522).
- 14) Magnetic structures in  $RNi_4B$  ( $R = Nd, Tb, Ho, Er$ ), E. Alleno and C. Mazumdar, *J. Solid State Chem.*, **202** (2013) 15 (Impact factor: 2.265 ; Times cited: 1).
- 15) Evidence of a structural phase transition in superconducting  $SmFeAsO_{1-x}F_x$  from  $^{19}F$  NMR, M. Majumder, K. Ghoshray, C. Mazumdar, A. Poddar, A. Ghoshray, D. Berardan and N. Dragoe, *J. Phys.: Condens. Matter.*, **25** (2013) 025701 (Impact factor: 2.209 ; Times cited: 5).

### *Chapter in a book*

- 16) Interdependent valence behaviour of Rare-Earth ions in Metallic Perovskites and Related Structures, Abhishek Pandey, Chandan Mazumdar, and R. Ranganathan, *Rare Earths: New Research*, Ed. Zhaosen Liu, Nova Scientific Publishers, (Invited contribution) (2013), pp. 117-144.

### *Papers published in international conference/symposium proceedings*

- 17) Study of Magnetic Properties of  $Pr_{0.4}Ca_{0.6}Mn_{0.98}Cr_{0.02}O_3$  Manganite, Papri Dasgupta, B. Biswas, S. Mukherjee, Asok Poddar, and Chandan Mazumdar, *Advanced Science Letters*, **22** (2016) 154 ; *Proc. of the First International Conference on Emerging Materials: Characterization and Application (EMCA-2014)*, 4-6 December, 2014, Kolkata, India.
- 18) Magnetic Relaxation Behaviour In  $Pr_2NiSi_3$ , Santanu Pakhira, Chandan Mazumdar and R. Ranganathan, *AIP Conf. Proc.* **1728** (2016) 020056 ; *Proc. of International Conference on Condensed Matter and Applied Physics*, Bikaner, India, 30-31 Oct., 2015.
- 19) Magnetic properties of intermetallic compound  $Pr_2NiSi_3$ , Santanu Pakhira, Chandan Mazumdar and R. Ranganathan, *AIP Conf. Proc.* **1665** (2015) 130019 ; *Proc. of the 59<sup>th</sup> DAE Solid State Physics Symposium 2014* ; Tamilnadu, India, 16-20 Dec. 2014.
- 20) Crystal structure and transport properties of two new compounds:  $SmPt_3B$  and  $GdPt_3B$ , Sudipta Mondal, Chandan Mazumdar and R. Ranganathan, *AIP Conference Proc.*, **1536**, (2013) 823; *Proc. of the International Conference on Recent Trends in Applied Physics & Material Science (RAM-2013)*, 01-02 Feb., 2013, Bikaner, India.
- 21)  $Ru_2VAl$  and  $Ru_2VGa$ : Two New Heusler-type compounds, Sanchayita Mondal, Chandan Mazumdar and R. Ranganathan, *AIP Conference Proc.*, **1536**, (2013) 825; *Proc. of the International Conference on Recent Trends in Applied Physics & Material Science (RAM-2013)*, 01-02 Feb., 2013, Bikaner, India.



- 22) Antiferromagnetic ordering in  $\text{GdCo}_{0.17}\text{Sn}_2$  and  $\text{GdCu}_{0.17}\text{Sn}_2$ , Krishanu Ghosh, Chandan Mazumdar, R. Ranganathan and S. Mukherjee, *AIP Conference Proc.*, **1536**, (2013) 989; *Proc. of the International Conference on Recent Trends in Applied Physics & Material Science (RAM-2013)*, 01-02 Feb., 2013, Bikaner, India.

### Research Highlights:

In the last 5 years, our group has focused on studying the physical properties of new intermetallics compounds that may have potential to exhibit interesting properties. We have emphasized on those materials which are either not reported in literature so far, or those whose formation are only known. We have carefully chosen those compounds which have rather simple crystal structure, yet may have the possibilities of exhibiting various interesting properties. The cubic  $\text{GdPd}_3$  is one such material, where we have reported the discovery of novel multiple sign changes versus applied magnetic field of the MR. Generally, the study of magnetoresistance often considered to be having both the theoretical as well as immense practical significance due exhibition of colossal MR and giant MR in many materials. Recently, extremely large MR of millions of percents in semimetals has also been reported. Our studies on  $\text{GdPd}_3$  shows a very strong correlation between magnetic, electrical and magnetotransport properties. The magnetic structure in  $\text{GdPd}_3$  appear to be highly fragile since applied magnetic fields of moderate strength significantly alter the spin arrangement within the system – a behavior that manifests itself in the oscillating MR. Intriguing magnetotransport characteristics of  $\text{GdPd}_3$  are appealing for field-sensitive device applications, especially if the MR oscillation could materialize at higher temperature by manipulating the magnetic interaction through perturbations caused by chemical substitutions [Pandey *et al.*, *Scientific Reports*, **7** (2017) Article No. 42789].

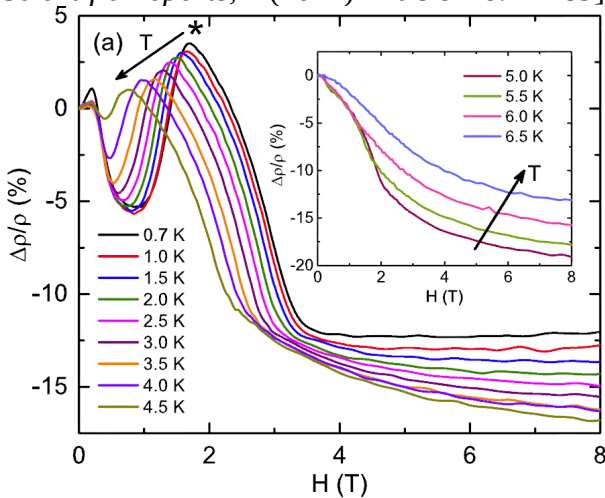


Fig: (a) Magnetoresistance  $\Delta\rho/\rho$  versus applied magnetic field  $H$  for  $\text{GdPd}_3$  measured at nine different temperatures  $T$  between 0.7 and 4.5 K. The peak with the highest positive MR is indicated with an asterisk. Inset:  $\Delta\rho/\rho$  versus  $H$  at four different  $T$ 's between 5 and 6.5 K. The arrows in the figure as well as in the inset indicate increasing temperatures of the isotherms.

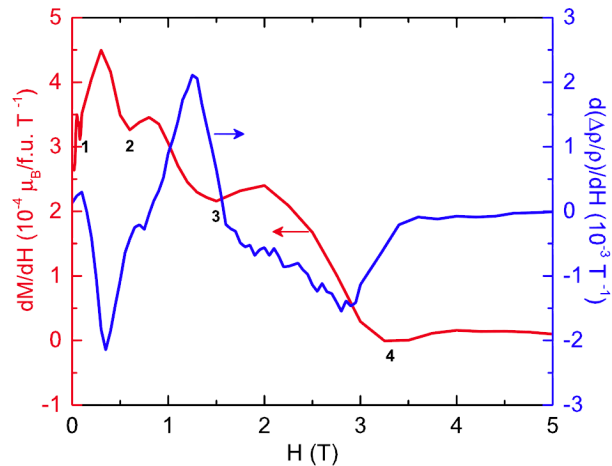


Fig: Magnetic field  $H$  derivative of the isothermal magnetization  $dM/dH$  versus applied magnetic field  $H$  of  $\text{GdPd}_3$  at 1.8 K (left ordinate) and the  $H$  derivative of magnetoresistance  $d(\Delta\rho/\rho)/dH$  versus  $H$  of  $\text{GdPd}_3$  at 1.5 K (right ordinate). Four distinct minima observed in the  $dM/dH$  versus  $H$  plot are indicated by numbers 1, 2, 3 and 4, respectively, in the order their occurrence with increasing  $H$ . The field derivative of the MR does not vary significantly between 1.5 and 2.0 K (not shown).

We have also worked on the physical properties of intermetallic antiperovskite  $\text{REPd}_3\text{B}$  ( $\text{RE}$  = rare earth) type of ternary compounds earlier. These compounds also form in cubic structure, where boron atoms occupy the body center position. However, plausibly due to the restricted space at the body center position, it was found that the occupancy factor for boron in these compounds is much less than 1. It was also reported that when Pd is replaced by larger sized Pt,  $\text{CePt}_3\text{B}$  can not

maintain its cubic phase and got converted to larger sized tetragonal structure that can accommodate B of full stoichiometry. This crystal got attention of the researcher after it was found that isostructural CePt<sub>3</sub>Si to be the first example of system that exhibit superconductivity in non-centrosymmetric system. Through our detailed research, we have shown that many members of REPt<sub>3</sub>B series of compounds can have both the tetragonal as well as cubic phase, while the boron stoichiometry in cubic phase is less than unity. This structural change is also associated with a substantially large volume reduction, rarely found in intermetallic or oxide compounds. Our findings is of quite importance as it opens a way to compare the physical properties of cubic and tetragonal phase so as to understand the controversial origin of unconventional superconductivity in isostructural CePt<sub>3</sub>Si [Mondal *et al.*, *Inorganic Chemistry* (2017) (accepted for publication)].

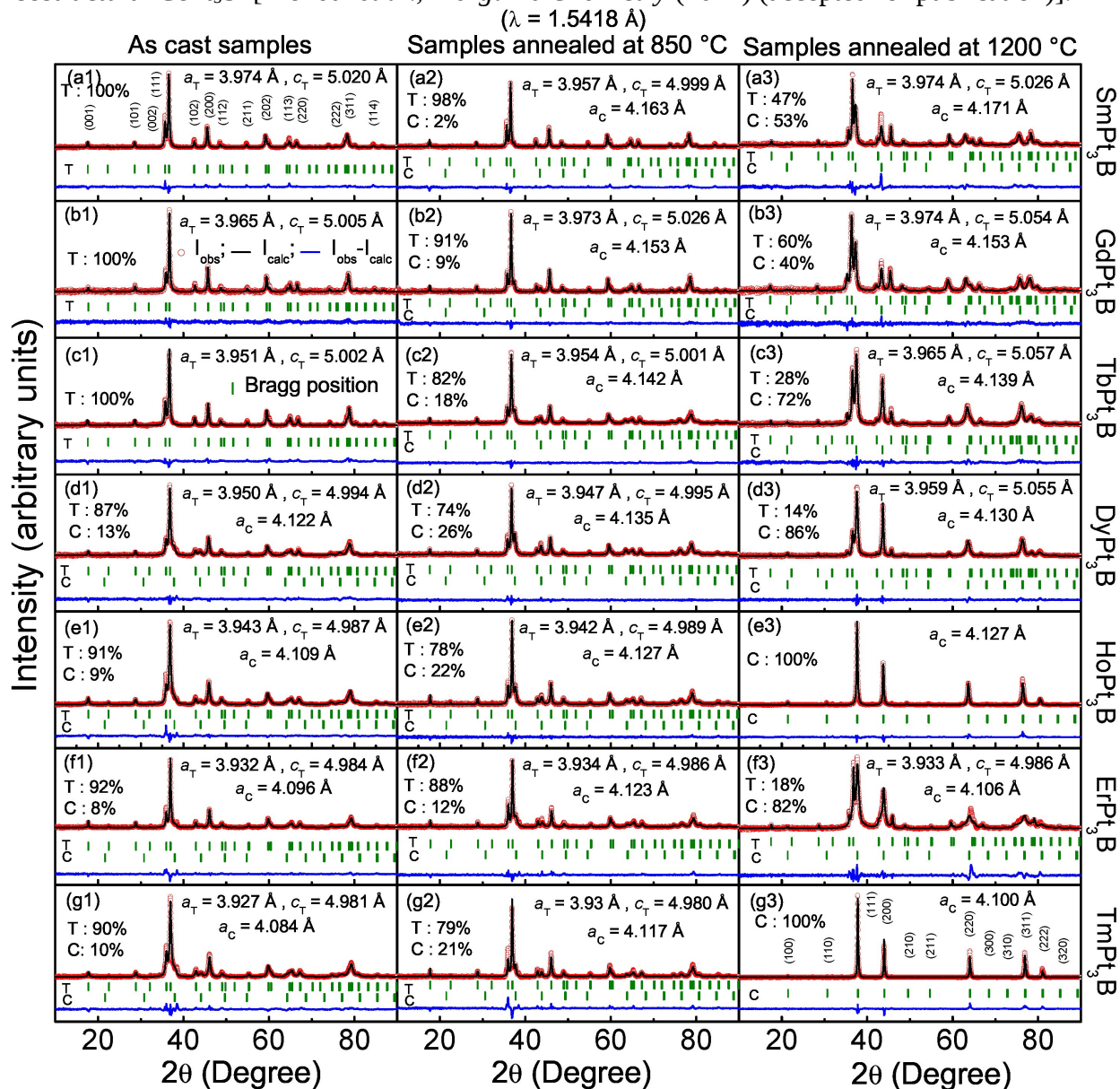


Fig: XRD analysis of REPt<sub>3</sub>B compounds. (A1-G3) Rietveld refinement of the powder XRD patterns at room temperature and calculated Bragg positions for space groups P4mm (T-panel) and Pm-3m (C-panel) of as-cast and annealed (at 850°C and 1200°C) REPt<sub>3</sub>B (RE = Sm, Gd-Tm) compounds.

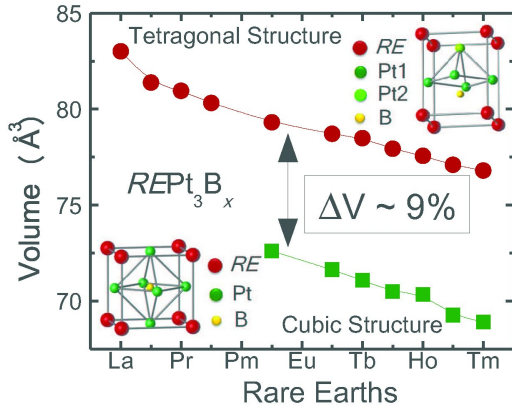


Fig:  $REPt_3B$  ( $RE = Sm, Gd-Tm$ ) compounds undergo an irreversible structural phase transformation from metastable high temperature (HT) tetragonal phase ( $REPt_3B$ ) to stable low temperature (LT) cubic phase ( $REPt_3B_x$ ) ( $0 < x < 1$ ) under annealing at high temperatures. This phase transition is associated with a considerably large volume reduction of  $\sim -9\%$  ( $\Delta c/c \sim -17\%$ ,  $\Delta a/a \sim +5\%$ )

The magnetically frustrated systems are another interesting subject, both from theoretical as well as technological point of view. The frustration may be of geometric in nature or may involve randomness of local environments. We have reported a non-stoichiometric intermetallic compound  $GdFe_{0.17}Sn_2$  (the paramagnetic Weiss temperature  $\theta_p \sim -59$  K) to exhibit the rare coexistence of a Griffiths phase (GP) and a geometrically frustrated (frustration parameter,  $f = |\theta_p|/T_N \sim 3.6$ ) antiferromagnetism. Normally Griffiths phase are reported either in ferromagnetic systems, or antiferromagnetic systems having with positive  $\theta_p$ . Except only one oxide system, no other antiferromagnetic compounds with negative  $\theta_p$  is ever reported to exhibit Griffiths phase behaviour. We have also shown that the Griffiths temperature,  $T_G$ , can also be determined through careful measurements of heat capacity as well magnetocaloric effect. In this work, we have also shown that substantial difference in GP region may exist between zero field and field cooled measurements - a fact hitherto not emphasized so far [Ghosh *et al.*, *Scientific Reports*, 5 (2015) Article No. 15801].

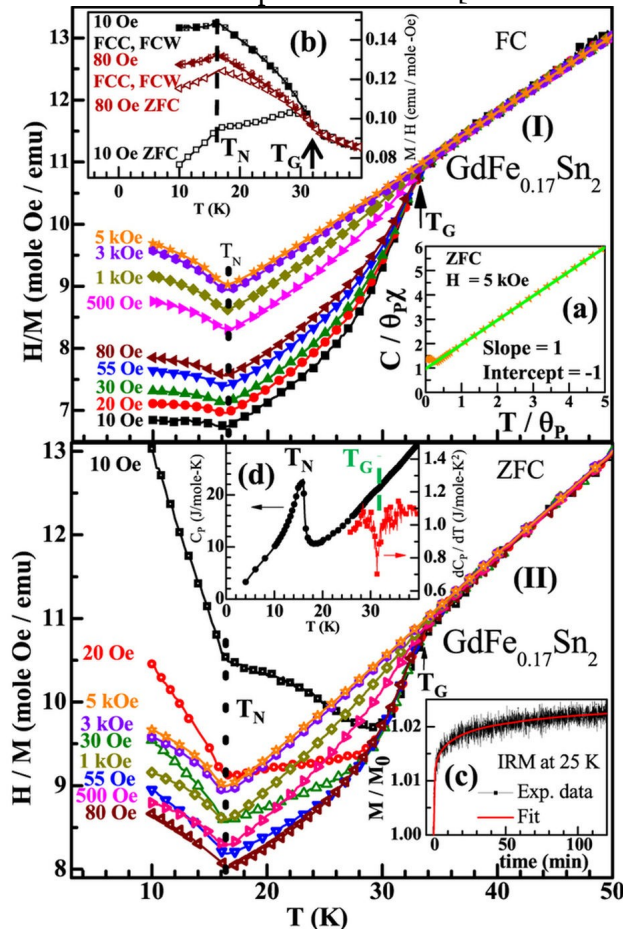


Fig: Temperature dependence of the inverse magnetic susceptibilities of  $GdFe_{0.17}Sn_2$  measured at different externally applied magnetic field under FC (top-I) and

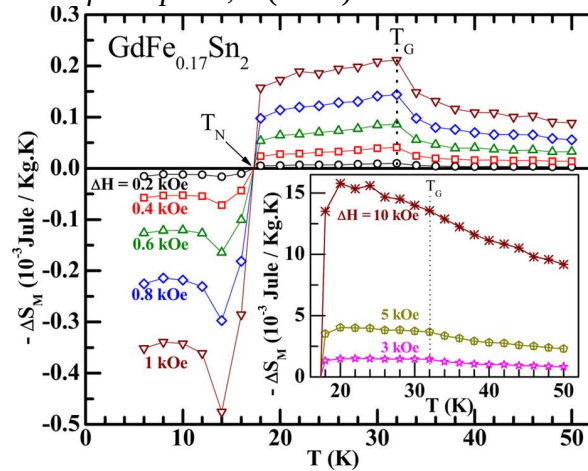


Fig: Magnetic entropy, estimated from low field isothermal magnetization measurements. (Inset): The magnetic entropy measured at higher magnetic fields.

ZFC (bottom-II) configuration during warming cycle (Inset (a)): Normalized inverse susceptibility versus temperature at  $H = 5$  kOe.  $C$  is the Curie constant and  $\theta_p$  is the paramagnetic Weiss temperature; (Inset (b)): Magnetic susceptibilities of the same sample measured under ZFC, FCC and FCW conditions in fields of 10 and 80 Oe; (Inset (c)): Normalized magnetic relaxation data along with the fit of stretched exponential are presented. (Inset (d)): Temperature dependence of heat capacity in absence of any magnetic field is shown using the left side axis. The anomaly observed due to GP transition can be observed more clearly by taking derivative of the heat capacity around TG as shown using the right hand axis of the inset.

As mentioned above, geometric frustration is not the only source of magnetic frustration observed in many compounds. For example, quite a few members of  $RE_2TMSi_3$  ( $TM = Cu, Rh, Pd, Pt$ ) are known to exhibit magnetic frustration. However, it was also found that most of the polycrystalline materials of the above series in generally formed with a few percent of secondary phase in the system. In our group, we have synthesized a new series of materials,  $RE_2NiSi_3$ , and shown that many of its members could be synthesized only in defect structure. Only  $Gd_2NiSi_3$  and  $Er_2NiSi_3$  could be synthesized in near stoichiometric form in single phase and we have studied their physical properties using dc magnetization, ac magnetic susceptibility, heat capacity, and neutron diffraction studies. Neutron diffraction and heat capacity studies confirm that long-range magnetic ordering coexists with the frustrated glassy magnetic components for both compounds. The static and dynamical features of dc magnetization and frequency-dependent ac susceptibility data reveal that  $Gd_2NiSi_3$  is a canonical spin-glass system, while  $Er_2NiSi_3$  is a reentrant spin cluster-glass system. A large magnetocaloric effect (MCE) is observed for both compounds. Maximum values of isothermal entropy change ( $-\Delta S_M$ ) and relative cooling power (RCP) are found to be 18.4 J/kg K and 525 J/kg for  $Gd_2NiSi_3$  and 22.6 J/kg K and 540 J/kg for  $Er_2NiSi_3$ , respectively, for a change in field from 0 to 70 kOe. The values of RCP are comparable to those of the promising refrigerant materials [Pakhira *et al.*, *Phys. Rev B*, **94** (2017) 104414].

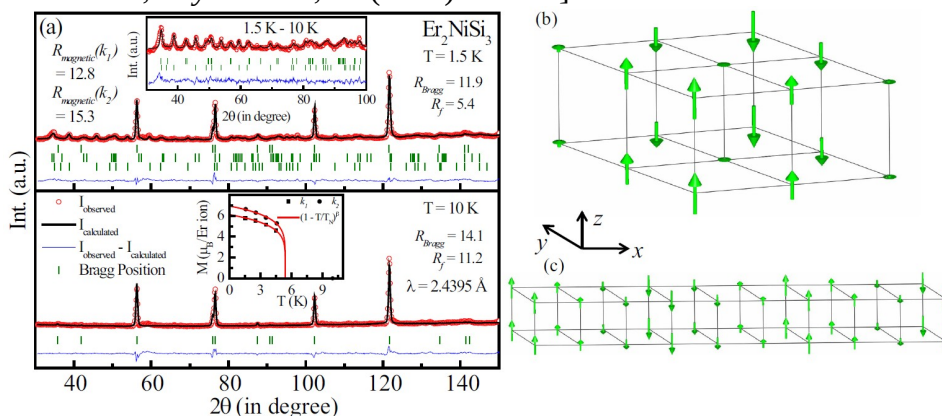


Fig: Zero-field neutron diffraction pattern of  $Er_2NiSi_3$  at  $T = 10$  K [lower panel, part (a)] and  $T = 1.5$  K [upper panel, part (a)] along with Rietveld refinement. The magnetic contribution of the diffraction pattern for  $T = 1.5$  K is shown in the inset of the upper panel of part (a). Temperature dependence of the ordered magnetic moments for the two magnetic phases are shown in an inset in the lower panel of part (a). The magnetic structures corresponding to propagation vectors  $k_1 = (0.1278, 0.1124, 0)$  and  $k_2 = (0.1634, 0, 0)$  are shown in (b) and (c), respectively.

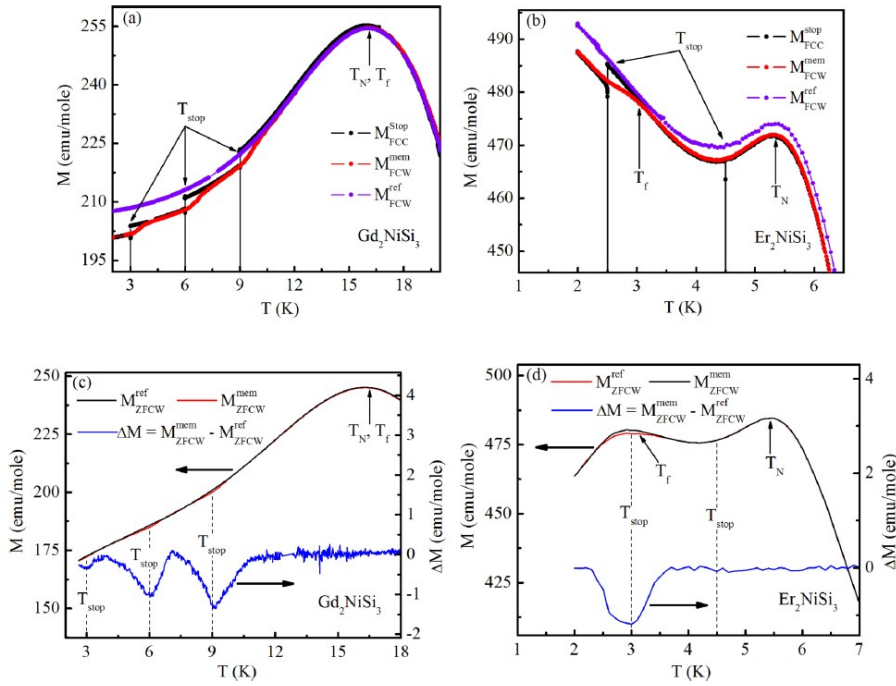


Fig: Memory effect of  $Gd_2NiSi_3$  in (a) FC and (c) ZFC protocol, as discussed in the text. Memory effect of  $Er_2NiSi_3$  in (b) FC and (d) ZFC protocol.

Among the non-stoichiometric compounds, we have seen that the Ho-analogue holds a special interest. The magnetic ground state of this material found to be highly frustrated without any long range order or glassy feature as investigated through magnetic, heat capacity and neutron diffraction measurements. The interest in this material stems from the fact that despite the absence of true long range order or spin freezing, large magnetocaloric effect (isothermal magnetic entropy change,  $-\Delta S_M \sim 28.65$  J/Kg K, relative cooling power, RCP  $\sim 696$  J/Kg and adiabatic temperature change,  $\Delta T_{ad} \sim 9.32$  K for a field change of 70 kOe) has been observed which is rather hard to find in nature. The absence of long range magnetic order indicates that the magnetic frustration is primarily responsible for large MCE in this compound. Such mechanism, although theoretically predicted earlier, had been rarely observed experimentally in any other systems.[Pakhira *et al.*, *Scientific Reports* (2017) (accepted for publication)].

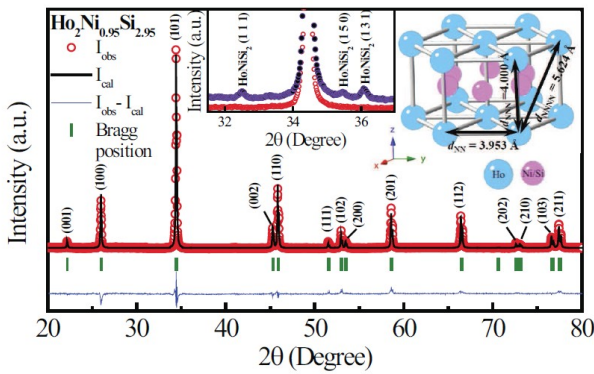


Fig: Room temperature XRD pattern of  $Ho_2Ni_{0.95}Si_{2.95}$  along with full Rietveld refinement. Inset shows the presence of  $HoNiSi_2$  type of secondary phase in  $Ho_2NiSi_3$  (violet), while  $Ho_2Ni_{0.95}Si_{2.95}$  (red) form in single phase. Crystal structure of  $Ho_2Ni_{0.95}Si_{2.95}$  is also displayed marked with nearest-neighbour distances.

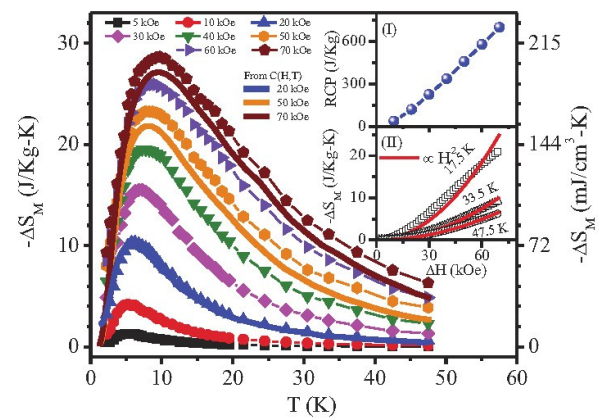


Fig: Temperature dependence of isothermal magnetic entropy change ( $-\Delta S_M$ ) at different field changes. Inset (I): Relative cooling power (RCP) as a function of applied field changes. Inset (II):  $H^2$  dependence of  $-\Delta S_M$  at different temperatures.

Beside the MCE, the magnetic ordering can also influence a few physical properties. There are even technical applications in finding zero-thermal expansion (ZTE) materials where the

magneto-volume effect can influence the temperature dependence of lattice parameters. For example, it was known that  $\text{Ho}_2\text{Fe}_{17}$  exhibits negative thermal expansion due to the effect of magnetic spin arrangements. Since zero thermal expansion has an immense application in many industries as well as many tools required in our daily life, we have attempted to achieve ZTE by weakening the magnetic interaction through non-magnetic element, Cr, substitution. We have shown that  $\text{HoFe}_{16}\text{Cr}$  exhibit ZTE in its volume over a very large temperature range 10-330K, covering the room temperature [Dan *et al.*, *RSC Adv.*, **6** (2016) 94809].

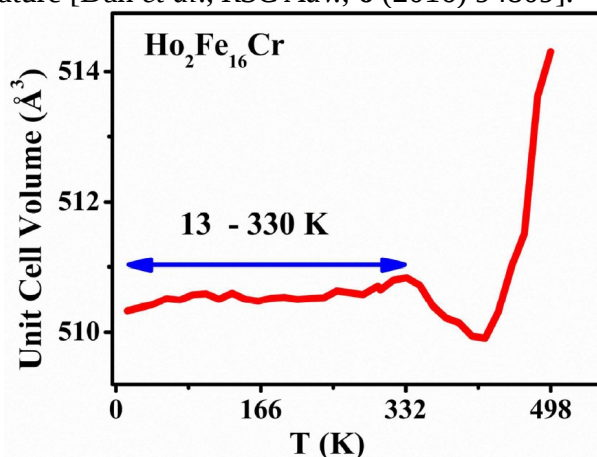


Fig:  $\text{Ho}_2\text{Fe}_{16}\text{Cr}$  with high  $T_c$ , moderate coercivity behaves like Zero Thermal Expansion Material in the temperature range 13 – 330 K.

In addition to intermetallics, we have also worked with a few oxide systems as well. For example, we have carried out an elaborate study on the magnetic properties and exchange bias phenomena of some charge-ordered (CO) manganites. The detailed study of  $\text{Sm}_{1-x}\text{Ca}_x\text{MnO}_3$  ( $x = 0.5, 0.55, 0.6, 0.65, 0.7$ ) compounds shows that  $\text{Sm}_{0.4}\text{Ca}_{0.6}\text{MnO}_3$ , which is the most robust charge ordered material in this series of compounds, shows significantly large exchange bias field ( $H_E$ ) as compared to the other compounds. Our experimental results and analysis also indicate that  $T_{\text{CO}}$ , which reflects the stability of the charge-ordered state, is one of the key parameters for the exchange bias effect. To find the generality of this behaviour, we have extended this study in other rare-earth analogues, viz.,  $\text{La}_{1-x}\text{Ca}_x\text{MnO}_3$  and  $\text{Pr}_{1-x}\text{Ca}_x\text{MnO}_3$  compounds as well. We found that with increasing stability of CO states in  $\text{Sm}_{1-x}\text{Ca}_x\text{MnO}_3$  compounds,  $H_E$  enhances due to increase in number and reduction in size of ferromagnetic clusters [Dasgupta *et al.*, *Scientific Reports*, **7** (2017) Article No. 3220].

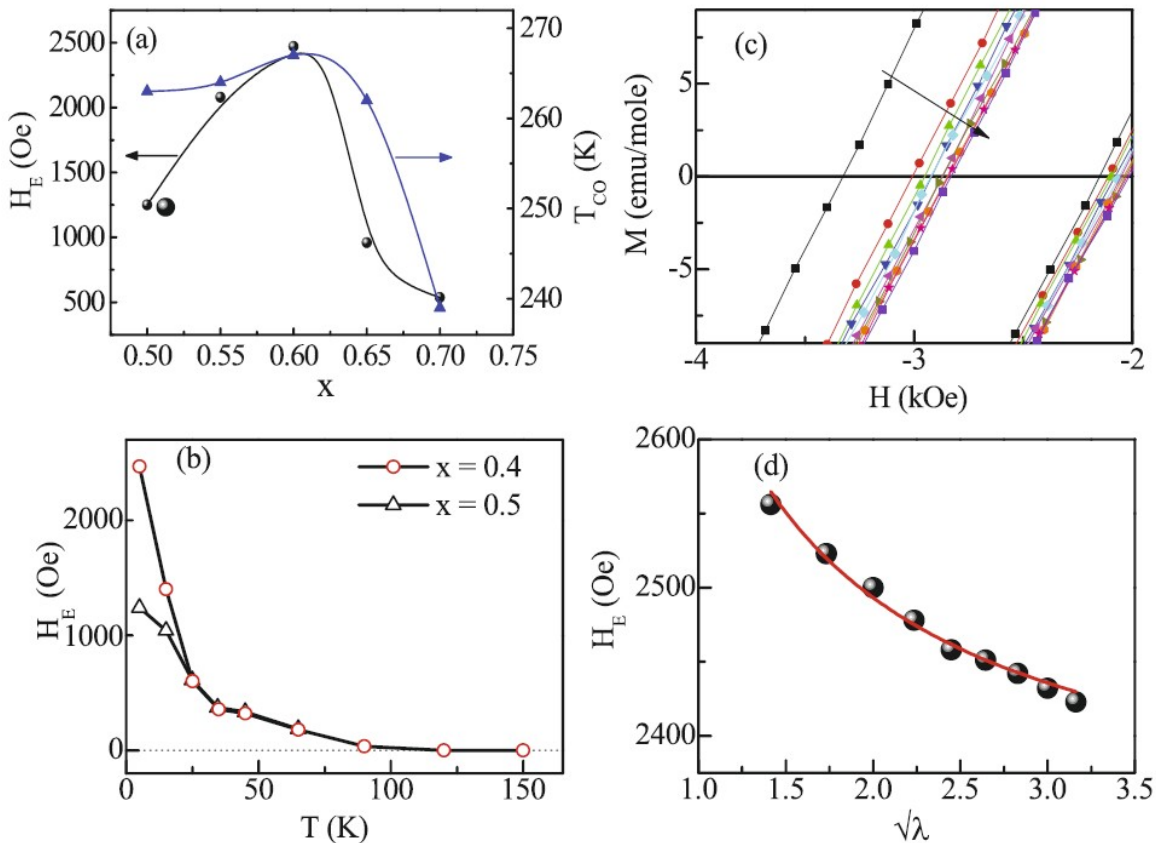


Fig: (a) Variation of  $H_E$  and  $T_{CO}$  as a function of Ca-concentration ( $x$ ). (b) Variation of  $H_E$  with temperature in bulk  $Sm_{1-x}Ca_xMnO_3$  compounds for  $x = 0.5$  and  $x = 0.6$ . (c)  $M(H)$  loops showing training effect of exchange bias and (d) Variation of  $H_E$  with the loop index number ( $\lambda$ ) in  $Sm_{0.4}Ca_{0.6}MnO_3$  compound.

### **Future directions:**

In coming years, we propose to complete the investigations of physical and magnetic properties of all these compounds. Among the intermetallic systems, we propose to study a few more similar new series, which are yet to be reported in literature. In some cases, preliminary studies have already been carried out to test the feasibility. Additionally, we also plan to study new systems with an aim to find new thermoelectric materials, which has an important effect on the power utilization effect, particularly power generation and refrigeration. This is one of the new field of research in which we would like to proceed in the near future. In the oxide series of compounds, we are particularly interested in double perovskite material as well as manganites. Both these type of compounds have been investigated for quite some time, but the high magnetic transition temperature, particularly above the room temperature, attract us towards its possible utilization in practical applications. One such application might be the zero thermal expansion, in addition to understanding many fundamental properties which still remain unsolved.

### **Important equipment and facilities:**

- A) Physical property measurement system; B) High temperature VSM with electromagnet;
- C) XRD system (Divisional In-charge)

## **INDRANIL DAS**

**Present Position: Sr. Professor 'H'** (from July 1<sup>st</sup>, 2016)

### **PhD students since 2012 (under my guidance)**

**(1) Name of Ph.D. Scholar:** Dr. Kalipada Das

**Title of Ph.D. thesis:** *Magnetic, Magneto-transport and Magnetocaloric Properties of Doped Perovskite Manganites*

Ph. D. degree in 2016 from The University of Calcutta, Dr. K. Das was selected for "Inspire Faculty" in 2017.

**(at present: Assistant Professor at S.A. Jaipuria Collage, Kolkata-700005)**

**(2) Name of Ph.D. Scholar:** Dr. Tapas Paramanik

**Title of Ph.D. thesis:** *Studies of Magnetic and Magnetocaloric properties in Intermetallic compounds*

Ph. D. degree in 2017 from The University of Calcutta.

**(at present: post-doctoral fellow at IIT Kharagpur)**

**(3) Name of Ph.D. Scholar:** **Mr. Sanjib Banik**

**Join CMP division for Ph.D. on August 2013**

**Title of Ph.D. thesis:** Study of Magneto-transport and Magnetocaloric Properties of Nano as well as Bulk Manganite Materials.

Thesis will be submitted within end of 2017

**(4) Name of Ph.D. Scholar:** **Mr. Snehal Mandal**

**Join CMP division for Ph.D. on August 2016.**

Ph.D. Program: Spin Caloric Transport & non local magnetoresistance in nanostructures

**(5) Name of Ph.D. Scholar:** **Mr. Apurba Dutta**

**Join CMP division for Ph.D. on August 2016.**

Ph.D. Program: Multiferroic properties in bulk and hybrid nanostructure materials.

### **External student:**

**(6) Name of Ph.D. Scholar:** **Mr. Suvayan Saha**

**Ph. D. Work Started in 2015,**

Ph.D. Topic : Magnetic, Magnetotransport and thermopower studies on oxide nanomaterials.

(INSPIRE FELLOW) Ph.D works under the joint guidance of Prof. Sudipta Bandyopadhyay (University of Calcutta) and I. DAS.



**Important equipment and facility under me:**

**(a) Cryogenic free Low temperature set-up with 9 Tesla Magnet:**



**(b) Versatile UHV thin film deposition set-up:**



**(c) Pulsed Laser Deposition setup (At present Laser source not working):**



### Conference/Symposium attended:

- i) (In recent years, I have received several invitations to deliver invited talks at many international conferences, but could not able to attend because of restrictions on foreign visit)
- Presented Invited Talk: *Giant enhancement of magnetoresistance in manganite nanostructures* at DAE- Solid State Physics Symposium (DAE-SSPS), December 21-25, 2015, Noida, New Delhi, organized by DAE.
- Presented Invited Talk: *Magnetoresistance and Magnetocaloric effect in Magnetic Nanostructures* at the 3rd Nano Technology conference "Bringing the Nanoworld Together" 24th - 25th November 2014, organize by Oxford Instrument at SINP. I also acted as the conference session chairman.
- Presented Invited talk: *Physics with nanostructured manganite materials* at the March meeting, March 7 - 8, 2013, School of Physical Sciences and Special Centre for Nanoscience of Jawaharlal Nehru University, New Delhi (theme of the symposium: Nanoscience -Condensed Matter Interface)
- Presented Invited talk: *Charge ordering in nanocrystalline manganites and its importance for magnetic field sensor at the KOLKATA MOSCOW SYMPOSIUM 22 – 23 January 2013* S.N. Bose National Centre for Basic Sciences, Kolkata

### Other academic records besides research and development (e.g. teaching)

#### **Project works Under my supervision: Post M.Sc review project 2015-16**

- (i) Project Title: **Spin Caloric Transport & non local magnetoresistance in nanostructure**  
Project Student: Mr. Snehal Mandal
- (ii) Project Title: **Multiferroic properties in bulk and hybrid nanostructure materials**  
Project Student: Apurba Dutta

#### **Project works Under my supervision: Post M.Sc review project 2013**

Project Title: **Magnetoelectricity in bi-layer thin film films and core shell nano-particles**  
Project Student: Mr. Sanjib Banik

#### **Supervised advanced experiment for the Post M.Sc. 2012 Student of SINP**

- (i) Post M.Sc Advanced experiment 2012: **Magnetic nanoparticle preparation and study**  
Post M.Sc. Students: (a) Achyut Maity, (b) Noasad Alam, (c) Sanjib Banik, (d) Anshu Chatterjee (e) Chitralkha Datta (f) Sukanta Barman
- (ii) Post M.Sc. Advanced experiment 2012: **Thin Film Multilayer Preparation by PLD and Characterization using AFM and X-ray Reflectivity**  
Post M.Sc. Students: (a) Tapas Ghosh, (b) Achyut Maity, (c) Noasad Alam, (d) Arpan Maiti

#### **Project works Under my supervision: Post M.Sc review project 2012**

- (i) Project Title: **Spin Caloric Transport**  
Project Student: Santu Manna
- (ii) Project Title: **Non Local electrical transport and non local magnetoresistance in nanostructure**  
Project Student: Sourav Kundu:

## **(B) Management, Administrative & Organizing Experience:**

### **Administrative work: 2014-15**

- ❖ Performed my duties as member of the Faculty Search Committee of SINP.
- ❖ I have taken part in the selection procedure of SINP research scholar.
- ❖ Performed my duties as member of the Budgetary Review committee of SINP.
- ❖ Performed my duties as member of the Workshop Committee.
- ❖ Performed my duties as member of the Canteen Committee.
- ❖ Acted as external expert in selection committee for scientist positions of S. N. Bose National Centre for Basic Sciences.
- ❖ Acted as external expert for the Interview Programme for the post of Research Associate at S. N. Bose National Centre for Basic Sciences.
- ❖ I have taken part in the selection procedure as external examiner of research scholar of IACS, Kolkata.
- ❖ Acted as external examiner for the Ph.D. Thesis defense of a research scholar of S.N. Bose Center.
- ❖ The international conference "Bringing the Nanoworld Together" (BTNT 2014) the 3rd Nano Technology conference was organized by Oxford Instruments (UK) on November 24-25, 2014 at SINP Kolkata with the active help from SINP. The conference had invited speakers, both in the field of basic and applied science from India and abroad, and technologists mainly from Oxford Instruments. A large number of young researchers had also participated. *I performed the responsibility as the local organizer of the conference.*

### **Administrative work: 2013-14**

- ❖ I have taken part in the selection procedure of SINP research scholar
- ❖ I have taken part in the selection procedure (as external examiner) of research scholar of IACS Kolkata.
- ❖ Performed my duties as member of Post M.Sc Teaching Committee.
- ❖ Performed my duties as member of Faculty Recruitment Committee open rolling advertisement (Evaluation Committee, Physics).

### **Administrative work: 2012**

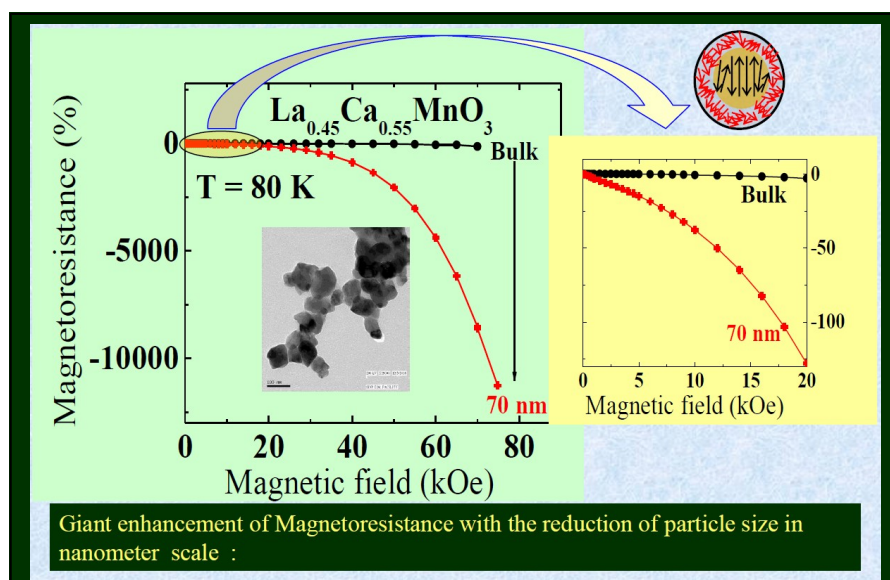
- ❖ I have taken part in the selection procedure of SINP research scholar.
- ❖ Performed my duties as member of Post M.Sc Teaching Committee.
- ❖ Responsible for distributing Post M.Sc student for advance experiment at various laboratory and arrangements for assessment.
- ❖ Performed my duties as member of Faculty Recruitment Committee open rolling advertisement (Evaluation Committee, Physics).
- ❖ Acted as External Examiner for evaluating the project dissertations and conducting the viva-voce examination of Dual-Degree M.Tech (final year students) and M.Tech students (2010-2012 batch) in the specialization SOLID STATE TECHNOLOGY. IIT, Kharagpur

## Significant Scientific contributions:

Some of our recent major findings from 2013 onwards (for which all planning, experiments & analysis were carried out under my guidance. Collaborative works are not mentioned here) are mentioned below:

### (1) Significant enhancement of magnetoresistance with the reduction of particle size in nanometer scale:

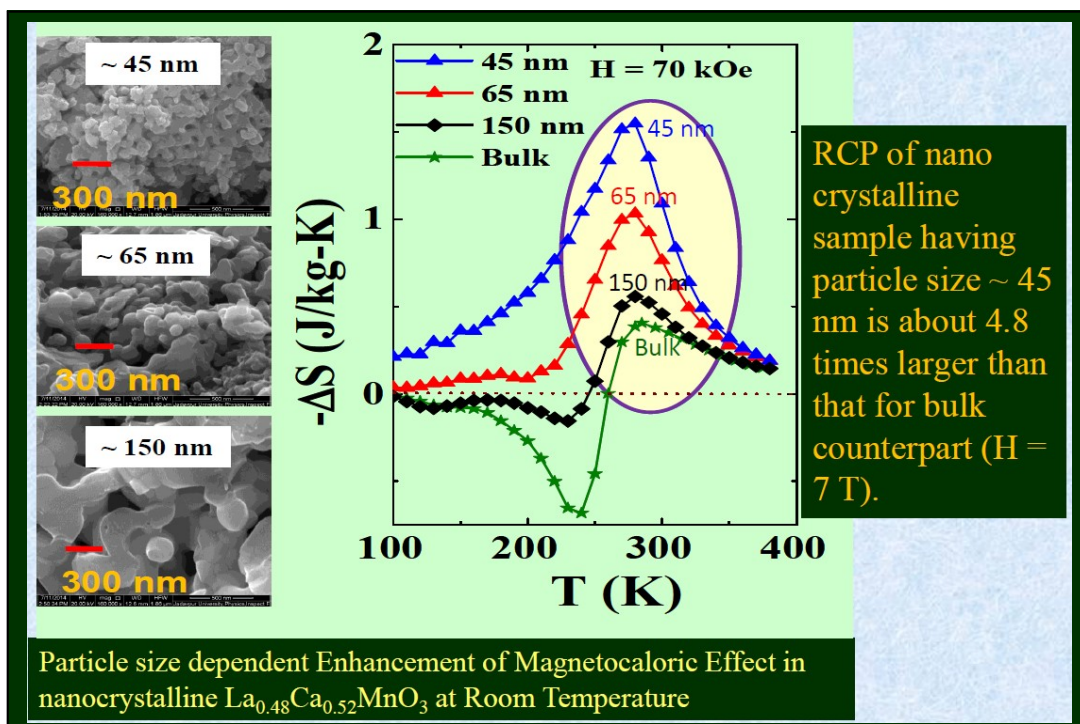
The Physics of materials with large magnetoresistance (MR; defined as the percentage change of electrical resistance with the application of external magnetic field) has been an active field of research for quite some times. In addition to the fundamental interest, large MR has widespread application that includes the field of magnetic field sensor technology. New materials with large MR is interesting. However it is more appealing to vast scientific community if a method describe to achieve many fold enhancement of MR of already known materials. We have shown a method for achieving the giant enhancement of magnetoresistance. Our study on several manganite samples [ $\text{La}_{1-x}\text{Ca}_x\text{MnO}_3$  ( $x = 0.52, 0.54, 0.55$ )] illustrates the method of giant enhancement of MR with the reduction of the particle size in nanometer scale. Our experimentally observed results are explained by considering model consisted of a charge ordered antiferromagnetic core and a shell having short range ferromagnetic correlation between the uncompensated surface spins in nanoscale regime. The ferromagnetic fractions obtained theoretically in the nanoparticles has been shown to be in the good agreement with the experimental results. The weakening of the charge-ordered state and the development of the short range ferromagnetic correlation between the uncompensated surface spins in nanoscale regime is the reason behind the phenomenon of huge enhancement of magnetoresistance. The method of several orders of magnitude improvement of the magnetoresistive property can have enormous potential for magnetic field sensor technology. The phenomenon appears to be wide spread in charge-ordered manganites.



Kalipada Das, P. Dasgupta, A. Poddar & I. Das  
**Scientific Reports (Nature Publishing Group) 6, 20351 (2016)**

## (2) Giant enhancement of magnetocaloric effect at room temperature by the formation of nanoparticle of $\text{La}_{0.48}\text{Ca}_{0.52}\text{MnO}_3$ compound:

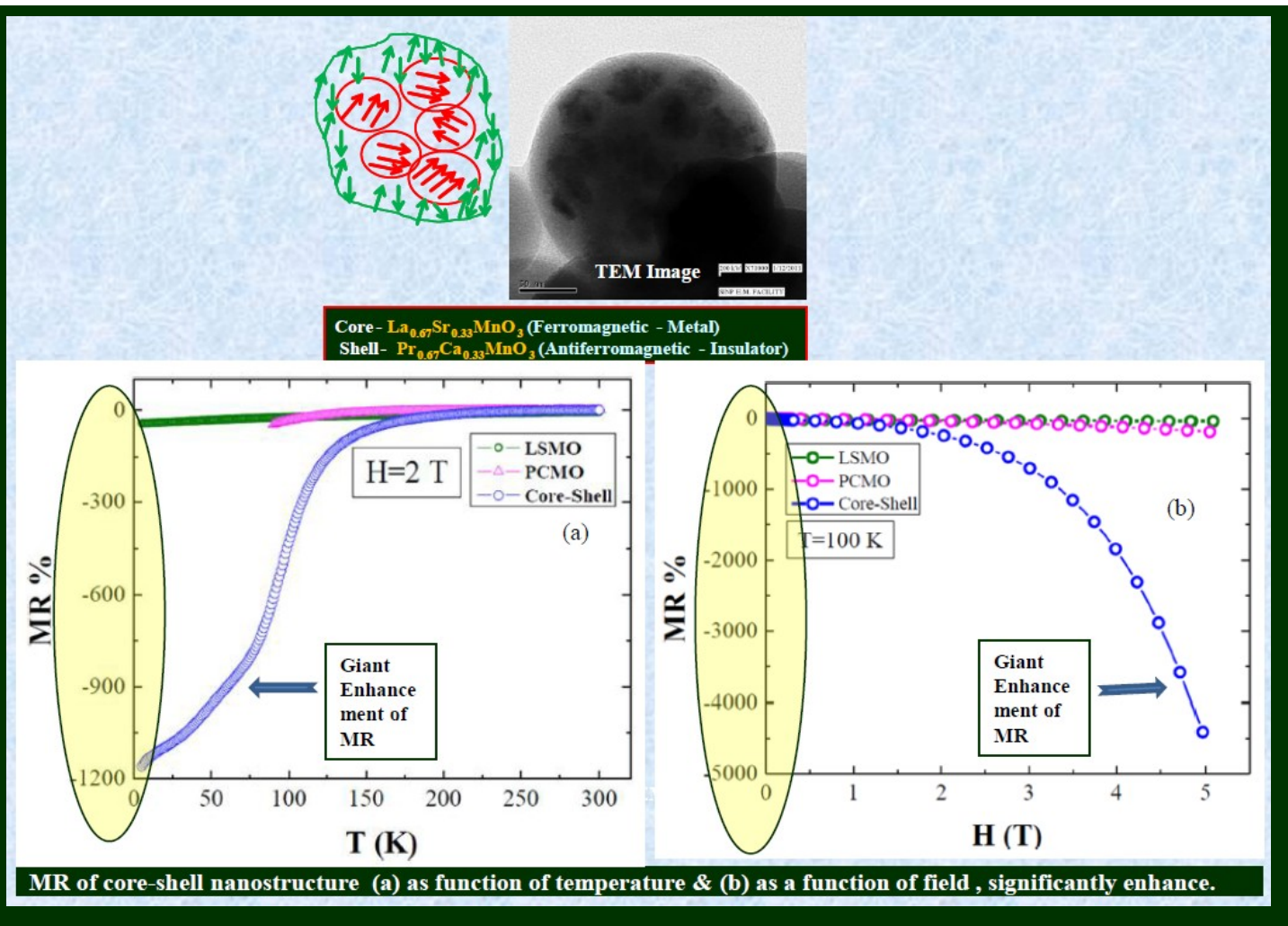
Magnetocaloric effect (MCE) is the change in temperature or magnetic entropy of a material due to the application of external magnetic field. The temperature dependence of MCE shows maximum value near the ferromagnetic transition of the material. Material with large MCE near room temperature will make revolutionary change in cooling technology and will have large impact in human society. We have shown that antiferromagnetic bulk  $\text{La}_{0.48}\text{Ca}_{0.52}\text{MnO}_3$  compound can be transformed to ferromagnetic material with the reduction of particle size in nanometer scale. Ferromagnetism is systematically enhanced with the reduction of particle size mainly due to the uncompensated surface spins. In addition to that in the nanoparticle compounds with large surface effect, the superparamagnetic nano clusters were formed even well above  $T_c$ . Our study reveals that not only the enhancement of magnetocaloric entropy change but also the relative cooling power at the room temperature increases to 4.8 times compare to the bulk counterpart for 45 nm particle size sample. It shows by the formation of nanoparticles of size few tens of nanometer of an existing bulk materials giant enhancement of relative cooling power is possible. It opens up a new direction of the already very active field research for the discovery of suitable material for future cooling technology.



Kalipada Das & I. Das  
J. Appl. Phys. (accepted, Feb'16)

### (3) Giant enhancement of magnetoresistance in core-shell ferromagnetic charge ordered nanostructures:

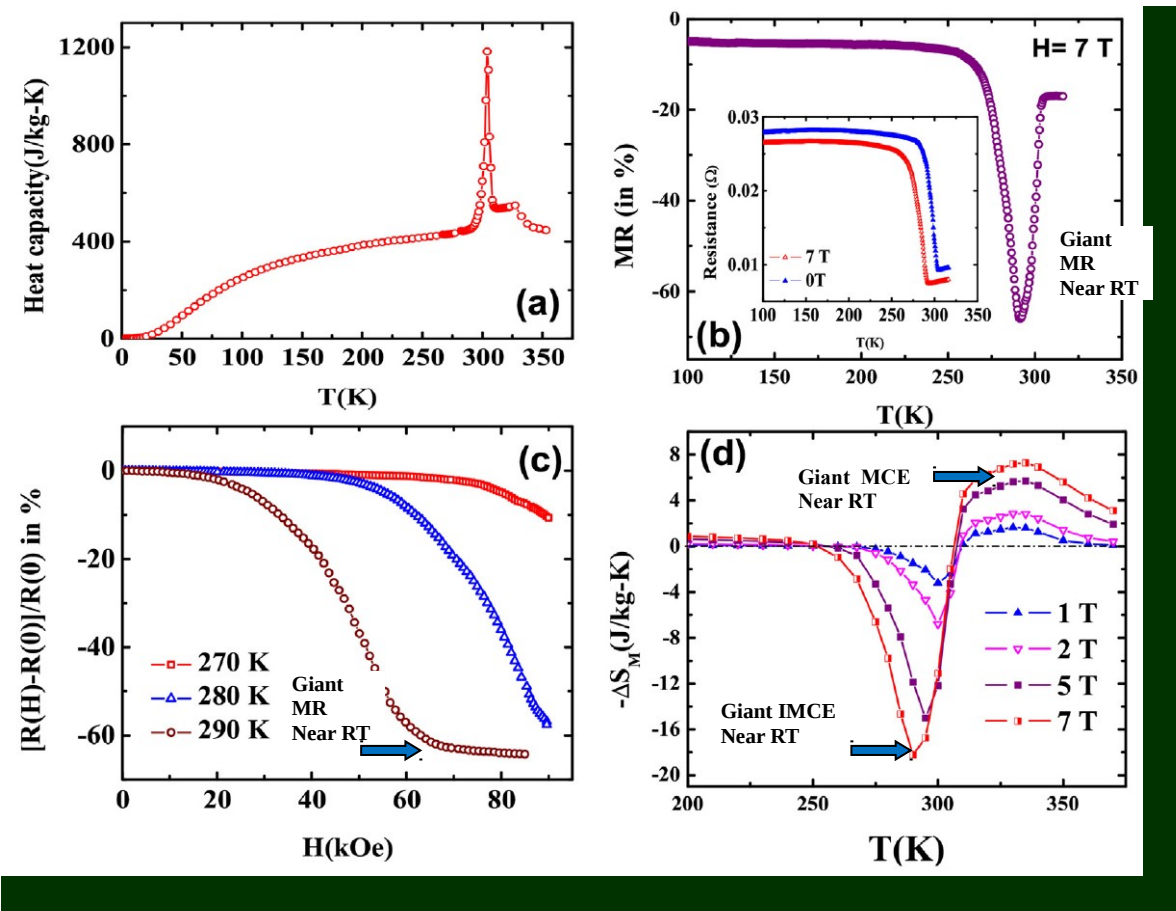
We have achieved giant enhancement of magnetoresistance (MR) by the formation of  $\text{La}_{0.67}\text{Sr}_{0.33}\text{MnO}_3$  (LSMO) –  $\text{Pr}_{0.67}\text{Ca}_{0.33}\text{MnO}_3$  (PCMO) core - shell nanostructure. Astonishingly, 1143% enhancement of MR in the core-shell nanostructure has been observed with respect to the parent PCMO nanoparticles at 100 K for 2Tesla and 2250% for 5 Tesla magnetic field value. The observed giant enhancement is the result of significantly weakened charge ordered state in the created ferromagnetic - charge ordered, core-shell nano structure. Our study clearly opens up a vast possibility of achieving gigantic enhancement of magnetoresistance by suitable combination of different materials in its nano form and fine tuning the relative proportion and size of the nano particle. The method of huge enhancement of magnetoresistance will eventually give rise artificially created superior materials important for magnetic field sensor technology.



Kalipada Das, R. Rawat, B. Satpati & I. Das  
*Appl. Phys. Lett.* **103**, 202406 (2013)

#### (4) Giant inverse magnetocaloric effect & giant magnetoresistance around room temperature in Co and Ga substituted Ni-Mn-In Heusler alloy

Giant magnetocaloric effect (MCE) and magnetoresistance near room temperature (RT) is very important, specially from technological point of view. First Order (FO) magnetostructural transition near RT can result giant magnetocaloric effect as well as large magnetoresistance. There is only a very few material families showing FO magnetostructural transition near RT and most of them are RE-based compounds like Gd-Si-Ge, La-Fe-Si etc. Recently there is a growing interest to discover RE free refrigerant materials and Heusler alloys that are believed to be the most promising and cost-effective material in that category. Ni<sub>50</sub>Mn<sub>50-y</sub>Z<sub>y</sub> based Heusler alloys (Z = In, Sn, Sb) have attracted great attention due to its multifunctional properties.



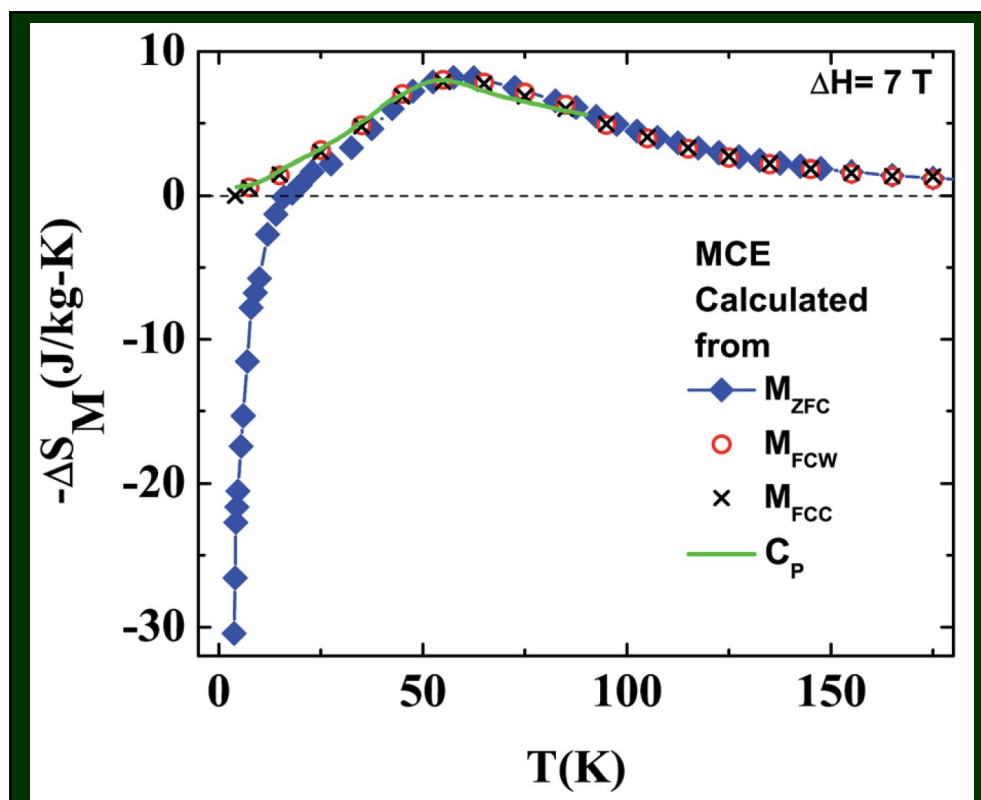
We have prepared the polycrystalline samples Ni<sub>48.4</sub>Co<sub>1.9</sub>Mn<sub>34.2</sub>In<sub>13.8</sub>Ga<sub>1.7</sub> by arc melting. With suitable substitution of Ni by Co and In by Ga, the martensitic transition temperature of Ni-Mn-In have been tailored to the room temperature. The structural, magnetic, magnetocaloric and magnetotransport properties of the doped Heusler alloy Ni<sub>48.4</sub>Co<sub>1.9</sub>Mn<sub>34.2</sub>In<sub>13.8</sub>Ga<sub>1.7</sub> have been studied in detail. Giant inverse magnetocaloric effect (IMCE) and giant negative magnetoresistance corresponding to the magnetostructural transition from austenite to martensitic phase around room temperature have been observed. The observation of both giant IMCE and giant negative magnetoresistance around room temperature makes this alloy very important rare-earth-free multifunctional material, potential for practical application in room temperature regime.

Tapas Paramanik & I. Das  
J. Alloys Comp. 654, 399 (2016)

## (5) Magnetic and magnetocaloric properties of Dy<sub>5</sub>Pd<sub>2</sub>: role of magnetic irreversibility

Magnetic behavior and magnetocaloric response of the intermetallic compound Dy<sub>5</sub>Pd<sub>2</sub> was investigated from detailed magnetization measurements. Magnetic cluster glass behavior was observed in the crystalline Dy<sub>5</sub>Pd<sub>2</sub> compound below 38 K. Magnetocaloric entropy changes (MCE) evaluated using Maxwell's relation (MXR) from zero-field-cooled (ZFC) magnetization isotherms. The most commonly used procedure of calculating MCE from ZFC magnetization measurement using MXR results in a giant inverse magnetocaloric effect (IMCE) below 20K as well as a large conventional MCE around 60 K ( $-\Delta S_M \sim 8$  J/kg-K for 7 Tesla field change) in this compound. The observed value of inverse MCE is as high as  $\Delta S_M \sim -38$  J/kg-K for 7 Tesla field change at  $T = 4$ K. In this context, the origin of the giant inverse MCE and its temperature dependence has been studied.

Our detailed analysis using FC magnetization and heat capacity data confirms that the giant IMCE observed in Dy<sub>5</sub>Pd<sub>2</sub> is due to magnetic irreversibility and the MC entropy change measured by commonly use method using MXR from ZFC magnetization data does not give a correct estimation of the reversible magnetic entropy change. The difference between the entropy changes measured using the ZFC and FC protocols reflects the irreversibility in the non-equilibrium magnetic behavior. Our study highlights the methodology needs to be followed for calculating the reversible magnetic entropy change which is the usable part for practical application using MXR from the FCW or FCC magnetization isotherms extracted from isofield magnetization curves.

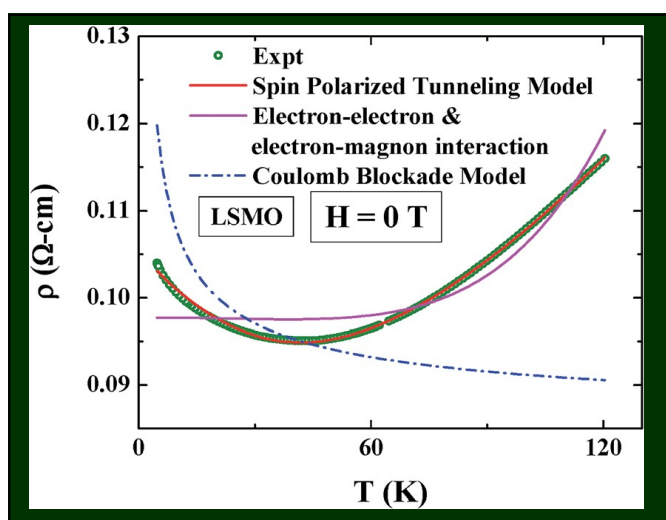
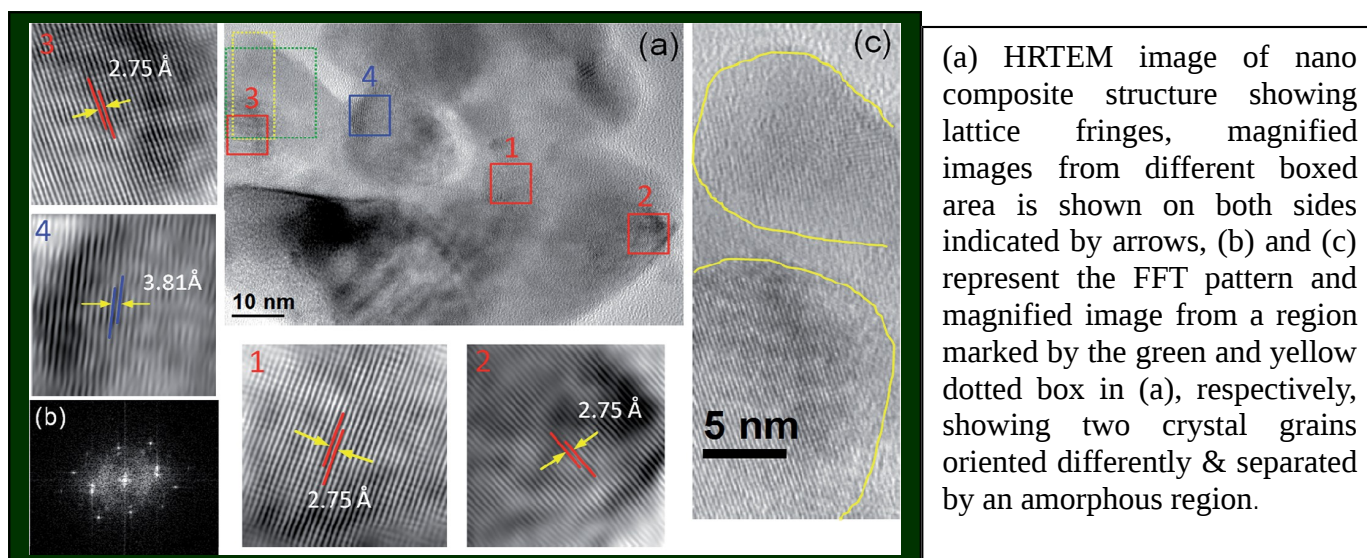


Magnetic entropy changes under a magnetic field change of 7 T obtained from the heat capacity and magnetization (under ZFCW, FCW and FCC protocols)



## (6) The effect of artificial grain boundaries on magneto-transport properties of charge ordered ferromagnetic nanocomposites

Nanocomposites of charge ordered insulating  $\text{Pr}_{0.67}\text{Ca}_{0.33}\text{MnO}_3$  (PCMO) and ferromagnetic metallic  $\text{La}_{0.67}\text{Sr}_{0.33}\text{MnO}_3$  (LSMO) nanoparticles have been prepared by chemical synthesis. Transport and magneto-transport properties of nanocrystalline LSMO and the PCMO–LSMO nanocomposites have been studied in detail. At a low temperature region, upturn of resistivity for both the compounds was observed. The upturn of resistivity is strongly influenced by the external magnetic field. The results are analyzed considering intergranular spin polarized tunneling model. Our study reveals that spin polarized tunneling (SPT) is the dominant mechanism leading to the rise in resistivity especially below  $T = 60$  K. It also indicates that SPT through the grain boundary is significantly modified in nanocomposite compounds, which leads to the enhancement of magnetoresistance and low field magnetoconductance compared to LSMO nanoparticles



K. Das, B.Satpati & I. Das  
RSC Adv. 5, 27338 (2015)

## (7) Resistivity minima in the disordered cluster glass intermetallic compound Dy<sub>5</sub>Pd<sub>2</sub>: influence of quantum interference effects

The polycrystalline intermetallic compound Dy<sub>5</sub>Pd<sub>2</sub> has been investigated by structural, magnetic, heat capacity and electrical resistivity measurements. Very interestingly a prominent minimum has been observed in the temperature dependence of the electrical resistivity around 60 K of the concentrated heavy rare earth Dy<sub>5</sub>Pd<sub>2</sub> compound. Similar minima in the electrical resistivity were previously observed in some metals, where they were attributed to the Kondo effect or to the Magnetic super-zone energy gap effect due to incommensurate long range magnetic structure. Kondo effect is not possible in the Dy<sub>5</sub>Pd<sub>2</sub> system because in case of Dy the 4f orbital is deep inside the Fermi level. Our previous study shows Dy<sub>5</sub>Pd<sub>2</sub> is a cluster glass system with no signature of long range ordering and thus the occurrence of a magnetic super-zone gap is also not possible.

A  $T^{3/2}$  contribution to the resistivity is observed at low temperature ( $T < T_f$ ) and around the minimum. Our analysis of the resistivity data reflects the simultaneous presence of the  $T^{3/2}$  type of magnetic contribution due to the spin diffusive modes in cluster glasses and weak localization (WL) along with  $\sqrt{T}$  dependence from the e-e interaction effects. The contribution from WL effects to resistivity has been confirmed from the field dependence of magnetization and magnetoresistance measurements.

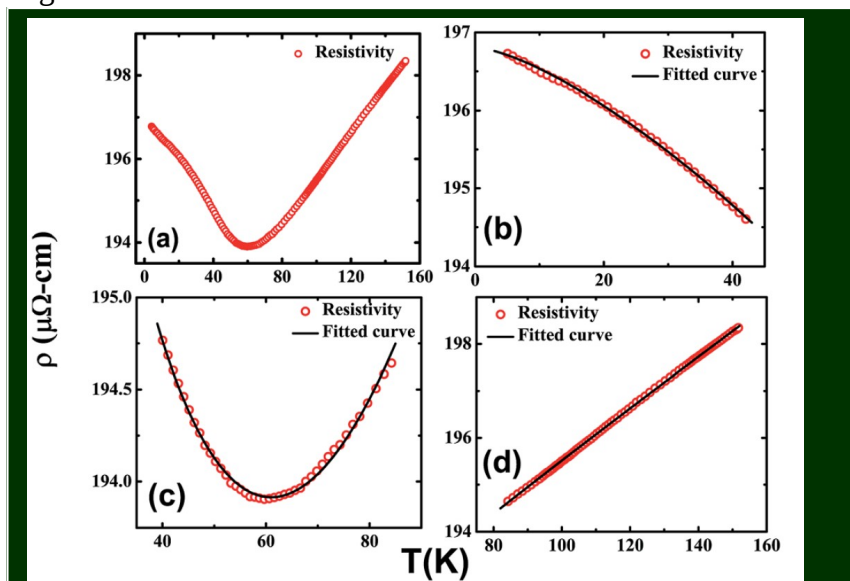
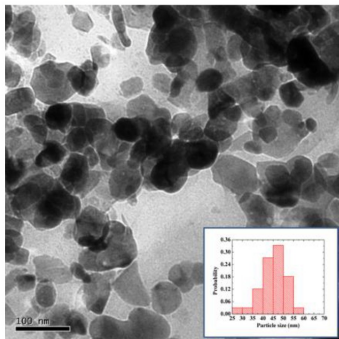


Figure highlights the resistivity minimum in the concentrated intermetallic compound Dy<sub>5</sub>Pd<sub>2</sub> that has been analyzed quantitatively in terms of electron–electron interactions, weak localization effects and magnetic contributions due to the cluster glass behavior.

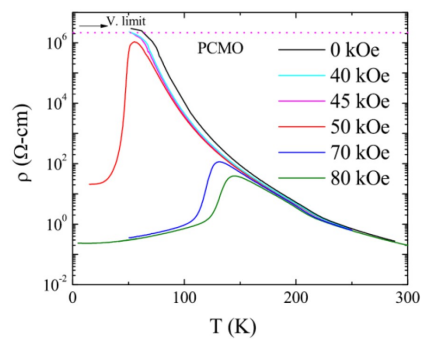
Tapas Paramanik & I. Das  
RSC Adv., 5, 78406, 2015

## **(8) Large field coefficient & temperature coefficient of resistance in nano crystalline $\text{Pr}_{0.67}\text{Ca}_{0.33}\text{MnO}_3$ compounds**

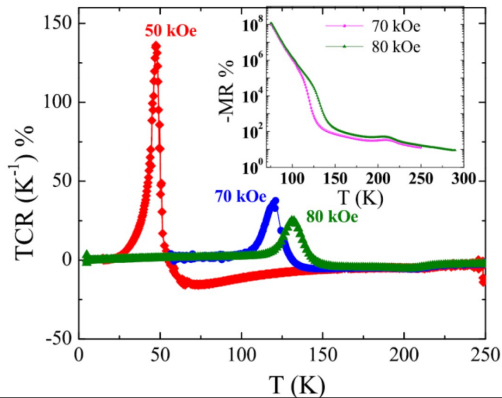
We have prepared nanocrystalline  $\text{Pr}_{0.67}\text{Ca}_{0.33}\text{MnO}_3$  compounds by sol-gel route with average particle size about 45nm. A magnetic field induced insulator-metal transition appears for the external magnetic field higher than 50 kOe. We have obtained very large value of the temperature coefficient of resistance (TCR) along with magnetoresistance and field coefficient of resistance (FCR). The value of TCR is 135%/K at 48 K. The calculated magnetoresistance is about  $-9.8 \times 10^7\%$  for 70 kOe and maximum FCR is about 320%/kOe around 75 K. Due to the application of the external magnetic field, charge ordered state of the compound is destabilized leading to such large values of TCR and FCR. Large values of TCR and FCR along with the large magnetoresistance exhibited by the nano material is very interesting from the application point of view.



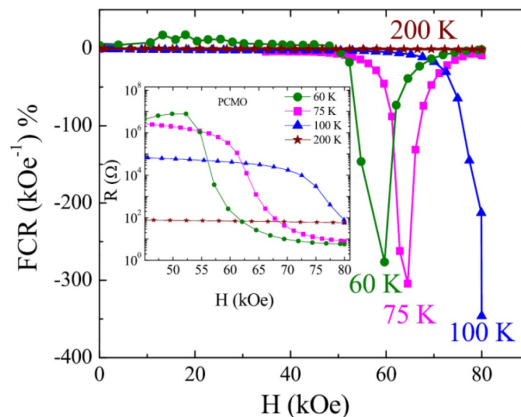
Transmission electron microscopy image of the nanoparticles of  $\text{Pr}_{0.67}\text{Ca}_{0.33}\text{MnO}_3$  compound. Inset shows the particle sizes distribution.



Temperature dependent resistivity at different magnetic fields. In the presence of  $H \geq 50$  kOe magnetic field, insulator-metal transition was observed at the low temperature region.



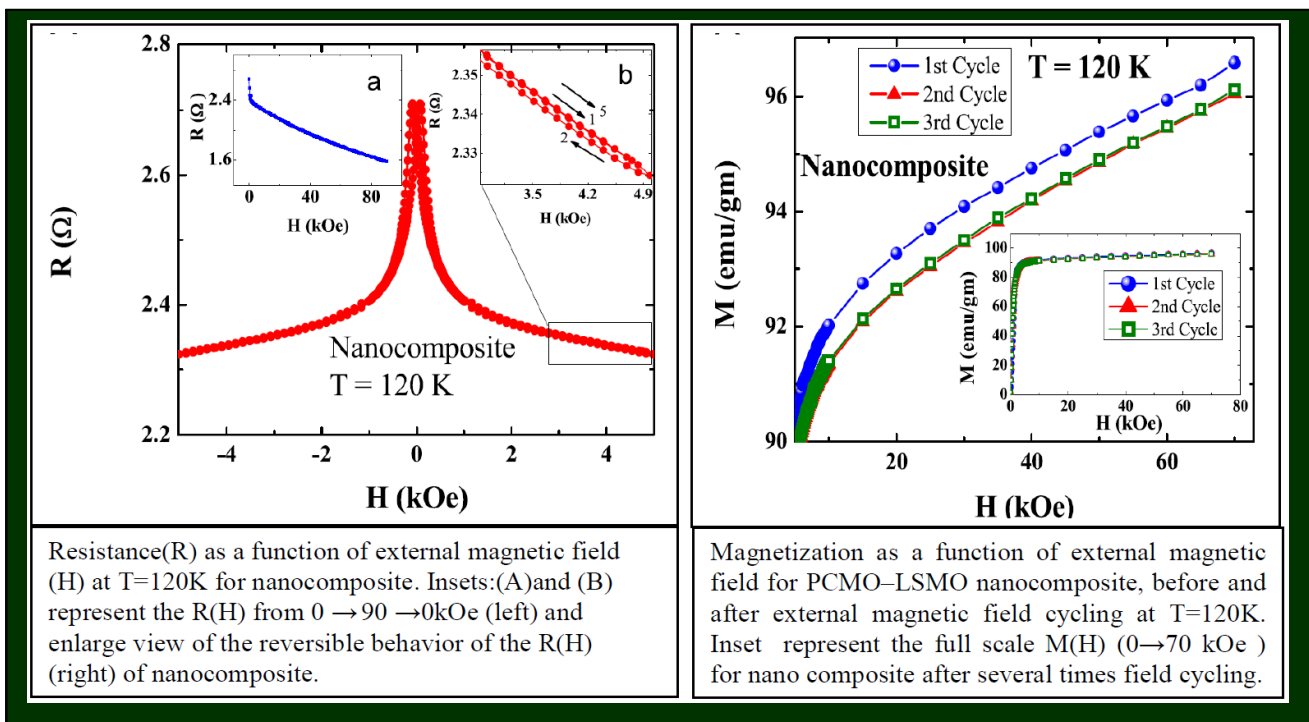
Temperature coefficient of resistance as a function of temperature for different magnetic field values. Inset of the figure indicates extremely large value of the magnetoresistance of the PCMO nanocrystalline compound.



Field coefficient of resistance as a function of the magnetic field at different temperatures. Inset represents the enlarged region of the magnetic field dependent resistances at several fixed temperatures.

## (9) Training effects induced by cycling of magnetic field in ferromagnetic rich phase-separated nanocomposite manganites

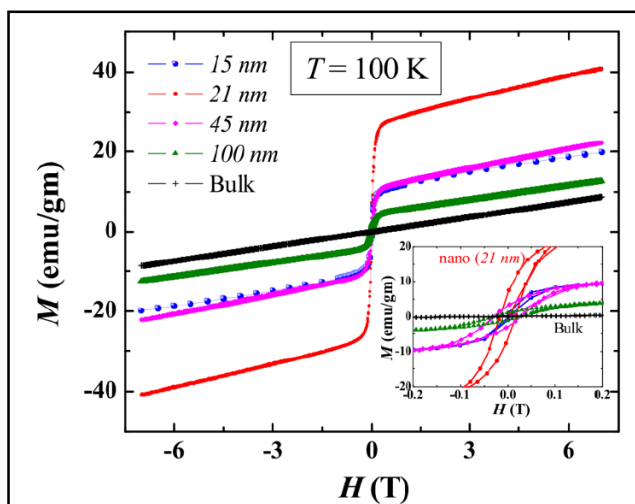
We have prepared charge-ordered anti-ferromagnetic  $\text{Pr}_{0.67}\text{Ca}_{0.33}\text{MnO}_3$  (PCMO)–ferromagnetic  $\text{La}_{0.67}\text{Sr}_{0.33}\text{MnO}_3$  (LSMO) nanocomposite as well as LSMO and PCMO nanoparticles by the sol–gel method. Experimental investigation of magneto-transport and magnetic properties were carried out. From the magneto-transport measurement no irreversibility was found due to the external magnetic field cycling for FM rich nanocomposite and LSMO nanoparticles. In contrast to the reversible magneto-transport results, our magnetization measurements indicate that the external magnetic field cycling induced training effect is present in phase separated nanocomposite and LSMO nanoparticles. As a result of the training effect the magnetization value is decreased due to the magnetic field cycling. The dissimilar behavior of magneto-transport and magnetic properties of phase separated compounds may be ascribed to the growth of the more perfect AFM domains with the external magnetic field cycling, keeping the ferromagnetic metallic percolation path for electrical transport unaltered.



Kalipada Das & I. Das  
**J. Mag. Mag. Mat. 395, 23 (2015)**

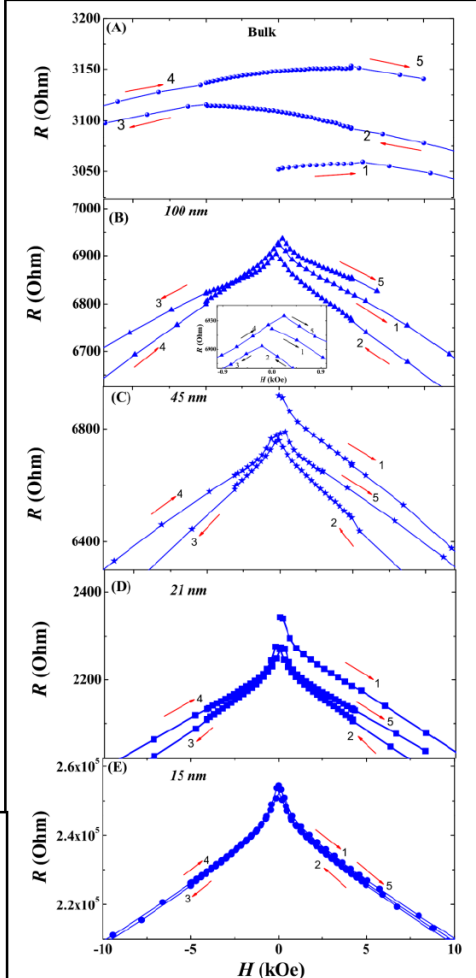
## (10) A comparative study of magnetic training effect in bulk and nano crystalline $\text{La}_{0.46}\text{Ca}_{0.54}\text{MnO}_3$ compound

We have studied the training effect of a charge ordered antiferromagnetic bulk and nanocrystalline  $\text{La}_{0.46}\text{Ca}_{0.54}\text{MnO}_3$  compound from transport, magnetotransport, and magnetic properties. The effect of the reduction of the particle sizes on magnetic field induced training effect has been investigated. By reducing the particle size, we have systematically increased the ferromagnetic counterpart and observed the striking correlation between charge ordering and training effect in nanocrystalline compound. By reducing the particle size, the charge ordering becomes gradually fragile and ultimately disappears in our lowest average particle size sample ( $\sim 15$  nm). Our measurements suggest that with the vanishing of the charge ordering signature in our lowest particle size sample, the signature of the training effect also becomes extinct. The study also brought out that the microscopic change of the magnetic state due to the magnetic field cycling may not be properly visualized from the magneto-transport measurements. However, the magnetic measurements indicate the more stable nature of the antiferromagnetic domain boundaries owing to the field cycling as it decreases the values of the hysteresis loops.



Magnetization hysteresis loop at  $T=100\text{K}$  for  $\text{La}_{0.46}\text{Ca}_{0.54}\text{MnO}_3$  compounds having different grain sizes. Inset indicates the clear view of hysteresis loops (enhanced ferromagnetic signature) with the reduction of the particle size.

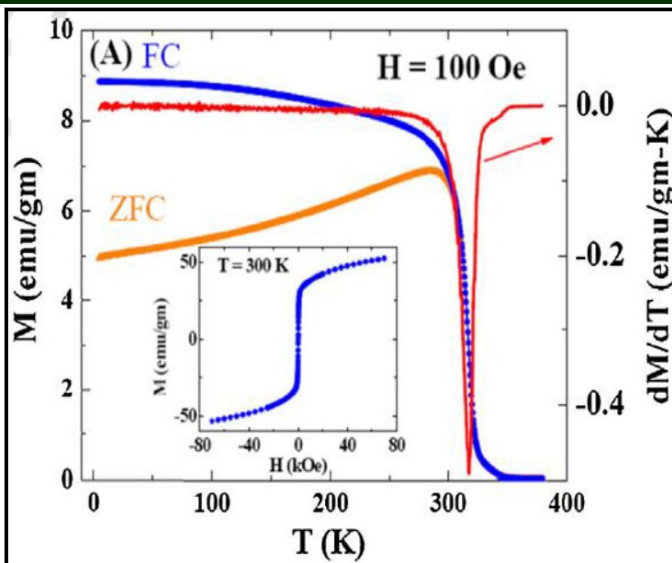
Resistance as a function of external magnetic field cycling (five quadrants) at  $T=100\text{K}$  for  $\text{La}_{0.46}\text{Ca}_{0.54}\text{MnO}_3$  compounds having different grain sizes. The presence of Magnetic training effect in bulk sample and the absence of the effect in  $15\text{nm}$  sample is highlighted in the figure.



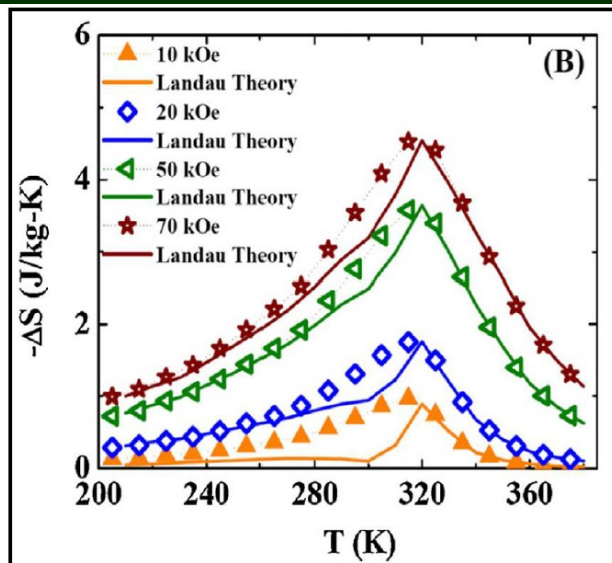
Kalipada Das & I. Das  
**J. Appl. Phys. 118, 084302 (2015)**

## (11) Large magnetocaloric effect near room temperature in polycrystalline $(\text{La}_{0.7}\text{Y}_{0.3})_{0.7}\text{Sr}_{0.3}\text{MnO}_3$ compound

We have studied detail magnetic and magnetocaloric properties of the polycrystalline compound  $(\text{La}_{0.7}\text{Y}_{0.3})_{0.7}\text{Sr}_{0.3}\text{MnO}_3$  prepared by sol-gel route. The compound undergoes a second order paramagnetic to ferromagnetic phase transition near the room temperature ( $T_c \sim 320$  K). We have achieved large magnetocaloric entropy change (MCE) with large relative cooling power (RCP) closed to the room temperature. The reduction of the tolerance factor and lattice contraction due to the 'Y' doping plays an important role for large RCP. For this large MCE and RCP, this compound may be suitable as a refrigerant material for future cooling technology. The magnetocaloric property of the compound has been analyzed considering Landau theory of magnetic phase transition.



Magnetization as a function of temperature measured in ZFC and FC protocol at  $H = 100$  Oe external magnetic field. The solid red line represents the first derivative of magnetization (FC protocol) indicates the paramagnetic to ferromagnetic transition temperature is  $T \sim 320$  K. Inset shows the negligible hysteresis at  $T = 300$  K.

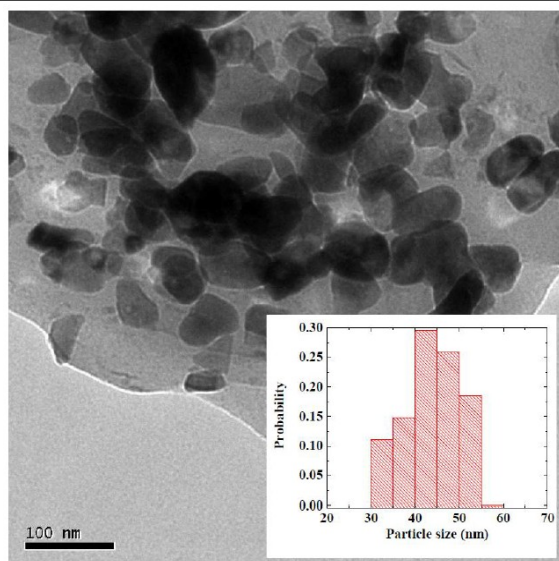


The magnetocaloric entropy change as a function of temperature for different constant magnetic field calculated from our experimental data as well as from Landau theory.

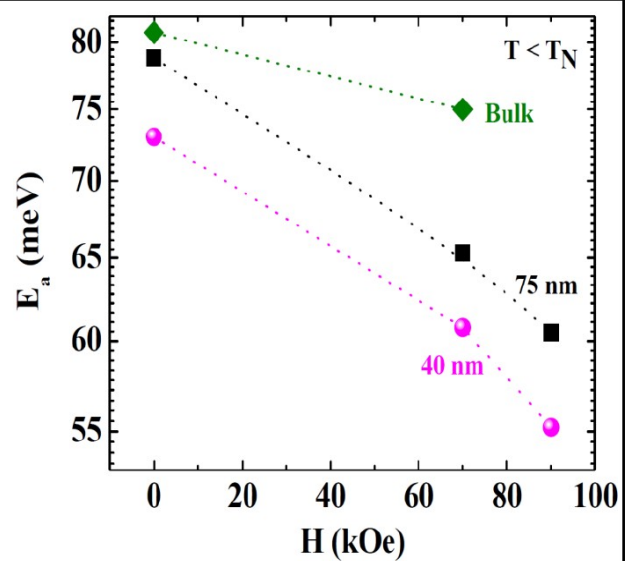
Kalipada Das, Sanjib Banik & I. Das  
*Mater. Res. Bull.* **73**, 256 (2016)

## (12) Size-induced modification of magneto-transport properties in nano-crystalline $\text{Sm}_{0.5}\text{Ca}_{0.5}\text{MnO}_3$ compound

we have studied the transport and magneto-transport properties of sol-gel prepared robust charge-ordered  $\text{Sm}_{0.5}\text{Ca}_{0.5}\text{MnO}_3$  compound in bulk and in nano forms having different average particles sizes. The insulating nature observed in transport and magneto-transport studies are analyzed by taking into account the adiabatic small polaron hopping model. Our experimental findings indicate that the insulating nature of  $\text{Sm}_{0.5}\text{Ca}_{0.5}\text{MnO}_3$  compound is found to reduce and the enhancement of magnetoresistance has been observed with the reduction of particle sizes. Our study reveals that in charge ordered manganite systems, there is a dependence of magnetoresistance on activation energy which modifies with the external magnetic field and particle size in nanometer scale.



Transmission electron microscopy image of the nanoparticles of SCMO compound having average particle size 40 nm. Inset shows the particle sizes distribution.

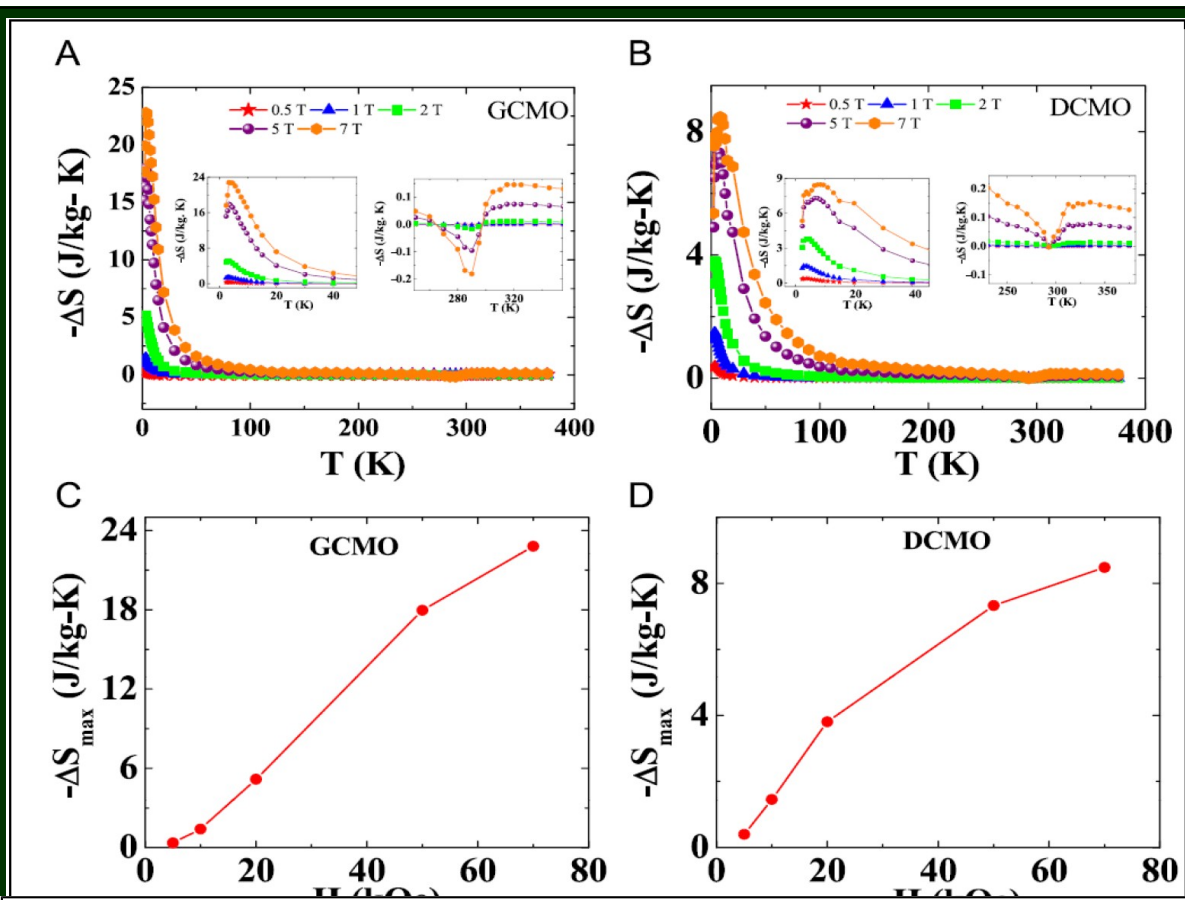


The variation of activation energy ( $E_a$ ) with the external magnetic field for different particle size samples of SCMO. Where activation energy ( $E_a$ ) was obtained by fitting the experimental resistivity data considering the expression of the resistivity below charge ordered state  $\rho(T) = AT \exp(E_a/K_B T)$  assuming the small polaron hopping model.

Sanjib Banik, Kalipada Das & I. Das  
*J.Magn.Magn.Mater.* **403**, 36 (2016)

**(13) Large magnetocaloric effect in  $\text{Ln}_{0.5}\text{Ca}_{0.5}\text{MnO}_3$  (Ln=Gd, DY) compounds: Consequence of magnetic precursor effect of rare earth ions**

Magnetic, specific heat and magnetocaloric studies have been performed on rare earth calcium manganites;  $\text{Gd}_{0.5}\text{Ca}_{0.5}\text{MnO}_3$  (GCMO) and  $\text{Dy}_{0.5}\text{Ca}_{0.5}\text{MnO}_3$  (DCMO). With lowering of temperature, both the compound goes from paramagnetic to charge order to canted magnetic state. In contrast to the generally observed large magnetocaloric effect around the paramagnetic to ferromagnetic transition temperature ; present study indicates that large magnetocaloric effect can also be observed at temperature well below the canted magnetic transition temperature due to the short range correlation developed in rare-earth ions at low temperature. The  $\text{Gd}_{0.5}\text{Ca}_{0.5}\text{MnO}_3$  compound for which charge ordering is around  $\sim 300\text{K}$  and goes to the canted state below  $\sim 150\text{K}$  shows large  $-\Delta S$  at  $4\text{K}$  (  $22.8\text{J/kgK}$  for  $70\text{ kOe}$  external magnetic field change). The large value of magnetic entropy change at the cryogenic temperature range for these compounds can also be interesting from application point of view.



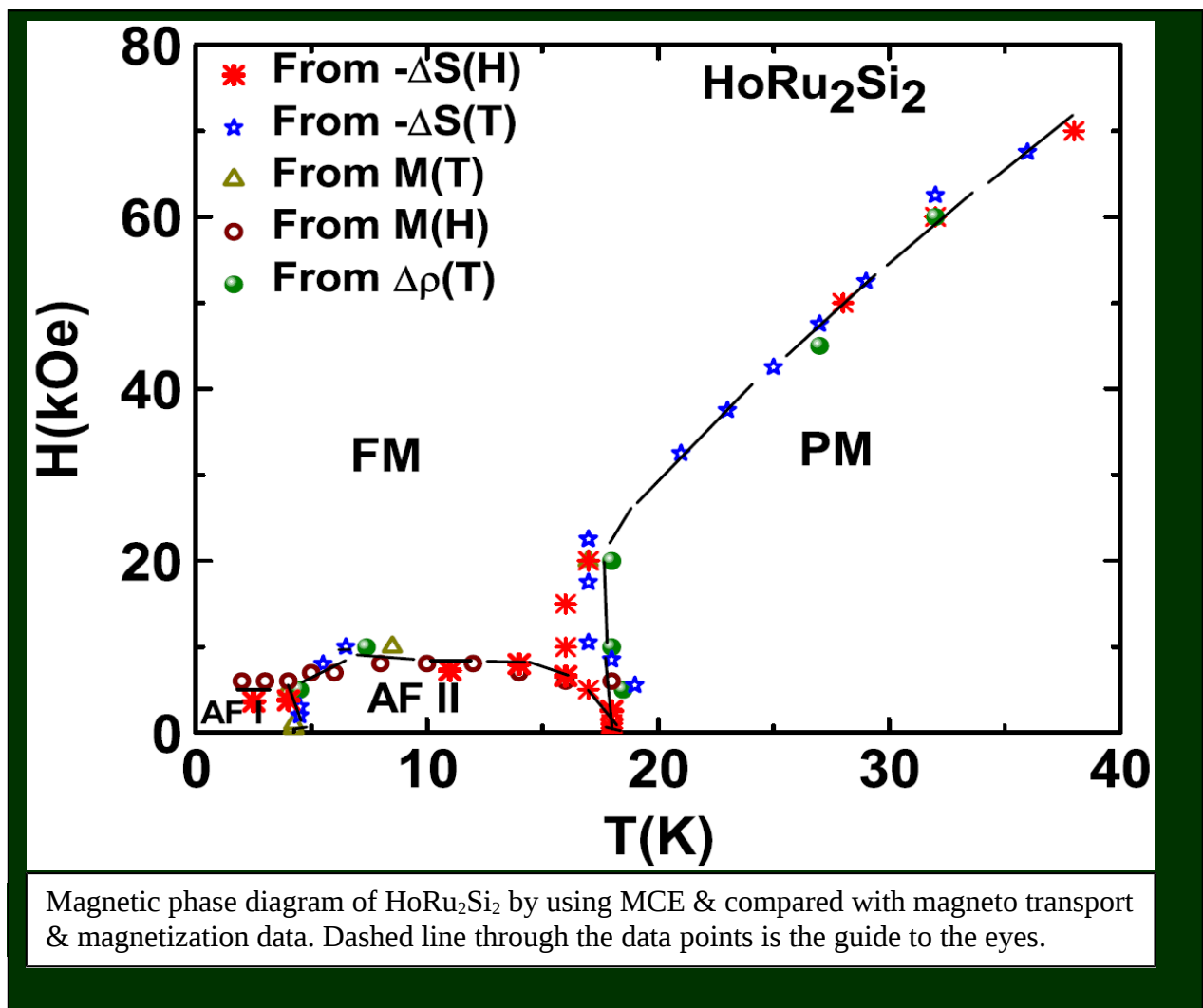
Isothermal magnetic entropy change as function of temperature at constant magnetic field for GCMO (A) and for DCMO (B). Variation of maximum magnetocaloric entropy changes with magnetic field for GCMO(C) and for DCMO(D) respectively. Insets of (A) and (B) show the enlarge portion of low temperature region and charge ordering region.

Kalipada Das, Tapas Paramanik & I. Das  
*J. Magn. Magn. Mater.* **374**, 707 (2015)



#### (14) Generation of magnetic phase diagram of HoRu<sub>2</sub>Si<sub>2</sub> using magnetocaloric effect

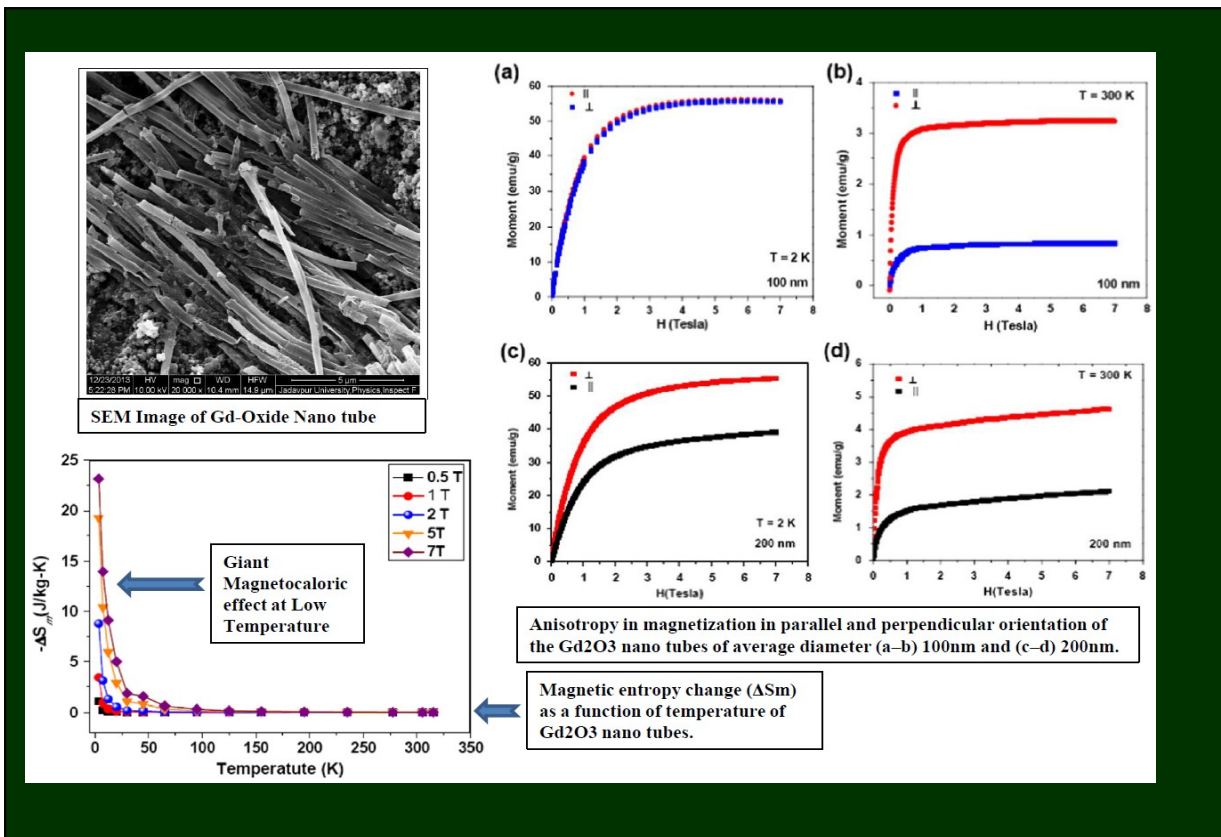
To get complete knowledge about the evolution of different magnetic phases on application of temperature and magnetic field magnetic, magnetotransport and magnetocaloric properties of HoRu<sub>2</sub>Si<sub>2</sub> have been investigated from 2 to 100K in magnetic fields ranging from 0 to 70kOe in detail. The complex magnetic phase diagram of HoRu<sub>2</sub>Si<sub>2</sub> has been generated by studying magnetocaloric effect (MCE). Three ordered phases have been observed. With lowering of temperature in the presence of lower magnetic field ( $H < 10\text{kOe}$ ) two different types of ordered antiferromagnetic phases have been observed. Both of the phases show metamagnetic transition on application of external magnetic field greater than the required critical field. An efficient procedure to construct magnetic phase diagram using MCE has been described. The overlap of the data points obtained from the magnetization and magnetotransport data at the phase boundaries with those generated by MCE indicates the strength of this powerful technique.



T. Paramanik, K. Das, T. Samanta & I. Das  
*J. Magn. Magn. Mater.* **381**, 168 (2015)

**(15) Magnetocaloric and anisotropic magnetic properties of Gd<sub>2</sub>O<sub>3</sub> nanotubes:**

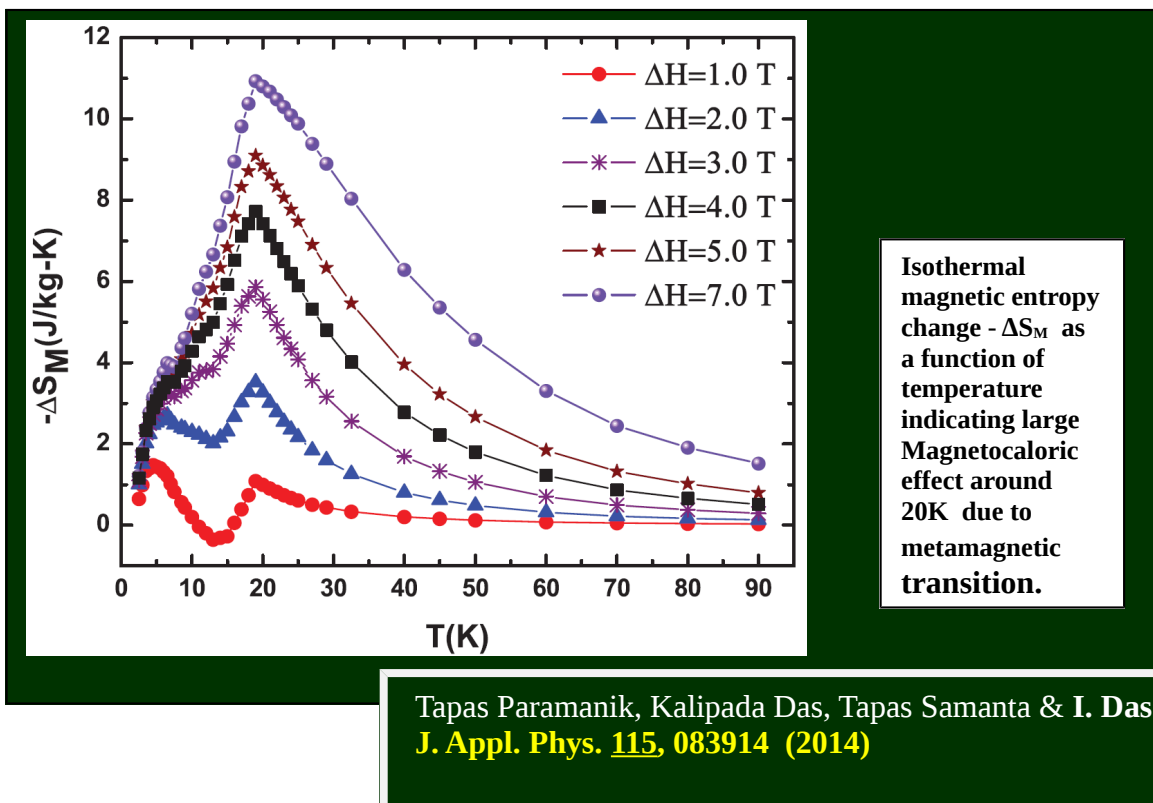
Gadolinium oxide (Gd<sub>2</sub>O<sub>3</sub>) nanotubes of micron length and average diameter 100 nm have been synthesized by a controlled template-assisted electrochemical deposition technique. Structure and morphology of the synthesized nanotubes have been well characterized by using microscopy and spectroscopy analyses. HRTEM and XRD analysis revealed the crystalline planes of Gd<sub>2</sub>O<sub>3</sub> nanotubes. Magnetic measurements of the aligned Gd<sub>2</sub>O<sub>3</sub> nanotubes have been performed for both parallel and perpendicular orientations of the magnetic field with respect to the axis of the Gd<sub>2</sub>O<sub>3</sub> nanotube array. Large bifurcation in ZFC-FC over the regime of 2-320 K without any signature of long range magnetic ordering confirms the presence of SPM clusters in Gd<sub>2</sub>O<sub>3</sub> nanotubes. Large magnetocaloric effect is observed in the cryogenic temperature regime. At low temperature region magnetic anisotropy is less for 100nm nanotubes, but it is found to evolve with temperature and becomes significant ~ 300 K. Giant magnetocaloric effect at low temperature has been observed.



Rima Paul , Pintu Sen & I. Das  
 Physica E **80**, 149 (2016)

## (16) Observation of large magnetocaloric effect in $\text{HoRu}_2\text{Si}_2$

Magnetocaloric effect (MCE) is the isothermal entropy change or change of temperature of magnetic materials when subjected to external magnetic field variation under adiabatic condition. Due to large energy-efficiency and environment friendly application over usual gas refrigeration technology, the search for new magnetocaloric (MC) materials is an attractive topic of research. Besides the MC materials with transition temperature near room temperature (RT) required for RT application, systems exhibiting large MCEs at cryogenic temperature are important because of their potential application in gas liquefaction. Detailed magnetic, magnetotransport, and magnetocaloric measurements on the  $\text{HoRu}_2\text{Si}_2$  intermetallic compound prepared by arc furnace have been performed. Presence of spin reorientation transition below paramagnetic to antiferromagnetic transition temperature ( $T_N = 19\text{K}$ ) has been observed. Our study shows due to the presence of field-induced spin-flip metamagnetic transition  $\text{HoRu}_2\text{Si}_2$  exhibits large, reversible magnetic entropy change  $9.1\text{ J/kg K}$  and large negative magnetoresistance  $\sim 21\%$  in a magnetic field of 5 tesla around  $T_N$ . The temperature dependence of all three parameters magnetization (M), magnetotransport, and MCE indicate occurrence of another magnetic phase transition below  $10\text{K}$ . The magnetic field dependence of M, MR, and MCE confirm this phase to be AFM in nature. The AFM compound  $\text{HoRu}_2\text{Si}_2$ , which exhibits a spin-flip transition, is a suitable candidate for magnetic refrigeration application around liquid hydrogen temperature. It is especially attractive because of large RCP of  $\text{HoRu}_2\text{Si}_2$ , large temperature span of cooling capability, minimum hysteresis effect, no bifurcation in temperature dependence of zero field cool (ZFC) and field cool (FC) magnetization, easy synthesis procedure, stability of the compound etc.



## **Future plan of I.DAS**

### **Title: Synthesis and Studies on Advance Energy Materials and Hybrid Quantum Structure:**

The group have made several important contributions in the field of Magnetocaloric effect. The group member have taken leading role for research on magnetocaloric effect in India. Magnetocaloric, Electrocaloric, Barocaloric effects are similar phenomena respectively arise in the response of external magnetic field, electric field and external presser on solid material that resulted significant change of temperature. Caloric materials, thermoelectric materials, energy storage materials, solar cell materials etc. are known as Energy Materials. The members of the group like to utilize their experience for the synthesis and studies on Energy materials.

Our group have specialize expertise in the field of magnetism and electrical transport as well as magnetic material synthesis both in low dimension and in bulk form. Our group have made several important findings in the field of magneto-transport\magnetoresistance. We like to develop hybrid low dimensional spintronic structure for the research on tunnel magnetoresistance, Giant magnetoresistance, Spin caloric effect, nonlocal magnetoresistance etc. and intended to make significant contribution in this technologically important field. We also like to develop hybrid structure of multiferroic materials, magnetic materials and topological insulators.

### **(1) Device structure fabrication and studies on Spin Caloric Transport:**

Spin caloric effect is an emerging new subfield of condensed matter physics concerned with coupled spin, charge, and energy transport in small structures and devices. Recent studies on spintronics and spin caloritronics *{Caloritronics => Spin + Calor → Heat + electronics}* have revealed that a spin current, a flow of spin angular momentum, is strongly coupled with a heat current in various magnetic systems. From both basic science and technological point of view, the interplay of these two currents is of crucial importance. With the recent discovery of fascinating spin-Seebeck effect *[a phenomenon enabling the conversion of heat currents into spin voltage]* or thermally driven spin injection, the highly efficient magnetization reversal by thermal-spin-torque etc. it is a very promising field of research.

### **(2) Research on Nonlocal electrical transport & nonlocal magnetoresistance in nanostructure:**

In contrast to local transport, Non-local transport implies voltage generation free of charge current. Non-local voltage measurement is an important tool to study spin current, spin accumulation etc. in spintronic devises. This is an emerging field of research with large technological and fundamental interest. Since very little is known about nonlocal effects various new findings in future can be expected. It is a very promising and frontline field of research. Before starting Ph.D. Work in this frontline topic during this project period this field of research will be reviewed to understand in detailed the experiments carried out in last few years and to understand the recent theoretical developments in this field.

### **(3) Studies on Spintronic materials, Spin Hall effect, & Device structure involving topological insulators:**

The spin Hall effect is a phenomenon arising due to spin-orbit coupling in which charge current passing through a sample leads to spin transport in the transverse direction. Key element of the spintronic device is spin polarized current which can be generated and detected by the spin hall effect. Spin current can be generated by the spin hall effect without magnetic field. It is a fundamentally exciting extremely frontline research topic. Since Spin Hall effect can generate dissipation less spin current it has tremendous technological interest because of its potential to develop new generation low power spintronic devices .

### **(4) Research on Multiferroic properties in bulk and hybrid nanostructure materials:**

### **(5) Mirror coating development for LIGO India:**

Development of appropriate coating materials for Laser interferometer-based gravitational wave detectors (for LIGO India) using dual ion beam sputtering deposition system.

#### **Any other relevant information:**

*During the period, 2010 to 2012, I was primarily devoted to develop new laboratory at old library space at the ground floor of SINP. Civil & Electrical works were done according to my instructions. I was involved in planning, placing order, installation, testing and rectifying problems of various experimental facilities that includes Cryogen-free low temperature set-up, Cryogen-free 9-Tesla magnet system, UHV thin-film deposition set-up etc. & associated set-ups.*



New Lab established during 2010-12 at SINP (Room No 140)

**I.DAS (CMP) Publications in Journals 2012-17**

<b>Sr. No</b>	<b>Names of the Authors</b>	<b>Total Number of authors  (Authors from SINP)</b>	<b>Title of the paper</b>	<b>Name of the Journal, volume, year, page</b>	<b>Journal Impact Factor</b>
1	Kalipada Das & I. Das	2 (2)	Large magnetoresistance and spin glass behavior of nanocrystalline La <sub>0.48</sub> Ca <sub>0.52</sub> MnO <sub>3</sub> compound at low temperature	<b>J. Magn. Magn. Mater.</b> <b>439</b> , 328, (2017)	2.0
2	Suvayan Saha, Kalipada Das, S.K Bandyopadhyay & I. Das	4(2)	A comparative study of magnetic field induced meta-magnetic transition in nanocrystalline and bulk Pr-0.65( Ca <sub>0.7</sub> Sr <sub>0.3</sub> ) 0.35MnO <sub>3</sub> compound	<b>J. Magn. Magn. Mater.</b> <b>432</b> , 271,, (2017)	2.0
3	Kalipada Das & I. Das	2 (2)	<a href="#">Magnetic and magnetocaloric properties of polycrystalline La<sub>0.48</sub>Ca<sub>0.52</sub>MnO<sub>3</sub> compound at low temperature: Influence of glassy magnetic state</a>	<b>Physica B</b> , <b>510</b> , 29 (2017)	1.5
4	Kalipada Das & I. Das	2 (2)	<a href="#">Magnetic and magnetoresistive properties of half-metallic ferromagnetic and charge ordered modified ferromagnetic manganite nanoparticles</a>	<b>J. Appl. Phys.</b> <b>121</b> , 103904 (2017)	2.2
5	Sanjib Banik, Kalipada Das, I. Das	3(3)	<a href="#">Enhancement of the magnetoresistive property by introducing disorder in the (La<sub>1-x</sub>Y<sub>x</sub>)<sub>(0.7)</sub>Ca<sub>0.3</sub>MnO<sub>3</sub> compound</a>	<b>RSC Adv.</b> , <b>7</b> , 16575, (2017)	3.8
6	Rima Paul, Tapas Paramanik, Kalipada; Das & I. Das	4(2)	<a href="#">Magnetocaloric effect at cryogenic temperature in gadolinium oxide nanotubes</a>	<b>J. Magn. Magn. Mater.</b> <b>417</b> , 182 (2016)	2.0
7	Rima Paul, Pintu Sen & I. Das	3(1)	<a href="#">Effect of morphology on the magnetic properties of Gd<sub>2</sub>O<sub>3</sub> nanotubes</a>	<b>Physica E</b> : <b>80</b> , 149 (2016)	2.0
	Sanjib Banik, Kalipada Das, I. Das		<b>6.</b> <a href="#">Size-induced modification of magneto-transport properties in nanocrystalline Sm<sub>0.5</sub>Ca<sub>0.5</sub>MnO<sub>3</sub></a>	<b>J. Magn. Magn. Mater.</b> <b>403</b> , 36 (2016)	2.0

			<a href="#">compound</a>		
8	<i>Kalipada Das &amp; I. Das</i>	2 (2)	Giant enhancement of magnetocaloric effect at room temperature by the formation of nanoparticle of $\text{La}_{0.48}\text{Ca}_{0.52}\text{MnO}_3$ compound	<b>J. Appl. Phys. <u>119</u>, 093903, 2016</b>	2.2
9	<i>Kalipada Das, P. Dasgupta, A. Poddar, &amp; I. Das</i>	4 (4)	Significant enhancement of magnetoresistance with the reduction of particle size in nanometer scale	<b>Scientific Reports (Nature Publishing Group) <u>6</u>, 20351 (2016)</b>	5.6
10	<i>Tapas Paramanik &amp; I. Das</i>	2 (2)	Near room temperature giant magnetocaloric effect and giant negative magnetoresistance in Co, Ga substituted Ni-Mn-In Heusler alloy	<b>J. Alloys and Compounds <u>654</u>, 399 (2016)</b>	3.0
11	<i>Kalipada Das, S. Banik &amp; I. Das</i>	3 (3)	Large magnetocaloric effect near room temperature in polycrystalline $(\text{La}_{0.7}\text{Y}_{0.3})_{0.7}\text{Sr}_{0.3}\text{MnO}_3$ compound	<b>Materials Research Bulletin, <u>73</u>, 256 (2016)</b>	2.3
12	<i>Rima Paul, PintuSen &amp; I. Das</i>	3 (2)	Effect of morphology on the magnetic properties of $\text{Gd}_2\text{O}_3$ nanotubes	<b>Physica E, <u>80</u>, 149 (2016)</b>	2.0
13	<i>Sanjib Banik, Kalipada Das &amp; I. Das</i>	3 (3)	Size-induced modification of magneto-transport properties in nanocrystalline $\text{Sm}_{0.5}\text{Ca}_{0.5}\text{MnO}_3$ compound	<b>J. Magn. Magn. Mater. <u>403</u>, 36 (2016)</b>	2.0
14	<i>Tapas Paramanik &amp; I. Das</i>	2 (2)	Resistivity minima in disordered cluster glass intermetallic compound $\text{Dy}_5\text{Pd}_2$ : Influence of quantum interference effects	<b>RSC Adv., <u>5</u>, 78406 (2015)</b>	3.8
15	<i>Tapas Paramanik Tapas Samanta, R Ranganathan, &amp; I. Das</i>	4 (3)	Magnetic and magnetocaloric properties of $\text{Dy}_5\text{Pd}_2$ : role of magnetic irreversibility	<b>RSC Adv., <u>5</u>, 47860 (2015)</b>	3.8
16	<i>Kalipada Das, B. Satpati, &amp; I. Das</i>	3 (3)	The effect of artificial grain boundaries on magneto-transport properties of charge ordered-ferro magnetic nanocomposites	<b>RSC Advances, <u>5</u>, 27338 (2015)</b>	3.8

17	<i>Kalipada Das, Tapas Paramanik &amp; I. Das</i>	3 (3)	Large magnetocaloric effect in $\text{Ln}_{0.5}\text{Ca}_{0.5}\text{MnO}_3$ (Ln = Gd, Dy) compounds: Consequence of magnetic precursor effect of rare earth ions	<b>J. Magn. Magn. Mater.</b> <b>374</b> , 707 (2015)	2.0
18	<i>T. Paramanik, Kalipada Das, T. Samanta &amp; I. Das</i>	4 (3)	Generation of magnetic phase diagram of $\text{HoRu}_2\text{Si}_2$ using magnetocaloric effect	<b>J. Magn. Magn. Mater.</b> <b>381</b> , 168 (2015)	2.0
19	<i>Kalipada Das &amp; I. Das</i>	2 (2)	Training effects induced by cycling of magnetic field in ferromagnetic rich phase-separated nanocomposite manganites	<b>J. Magn. Magn. Mater.</b> <b>395</b> , 23 (2015)	2.0
20	<i>Kalipada Das &amp; I. Das</i>	2 (2)	A comparative study of magnetic training effect in bulk and nanocrystalline $\text{La}_{0.46}\text{Ca}_{0.54}\text{MnO}_3$ compound	<b>J. Appl. Phys.</b> <b>118</b> , 084302 (2015)	2.2
21	<i>Kalipada Das &amp; I. Das</i>	2 (2)	Magnetic field induced insulator-metal transition in nanocrystalline $\text{Pr}_{0.67}\text{Ca}_{0.33}\text{MnO}_3$ compounds: Evidence of large temperature coefficient of Resistance	<b>J. Appl. Phys.</b> <b>117</b> , 17503 (2015)	2.2
22	<i>T. Paramanik, Kalipada Das, T. Samanta, &amp; I. Das</i>	4 (3)	Observation of large magnetocaloric effect in $\text{HoRu}_2\text{Si}_2$	<b>J. Appl. Phys.</b> <b>115</b> , 083914 (2014)	2.2
23	<i>V. K. Shukla, S. Mukhopadhyay, Kalipada Das, A. Sarma &amp; I. Das</i>	5 (3)	Direct experimental evidence of multiferroicity in a nanocrystalline Zener polaron ordered manganite	<b>Phys. Rev. B</b> <b>90</b> , 245126 (2014)	3.7
24	<i>A. Biswas, S. Chandra, T. Samanta, B. Ghosh, S. Datta, M. H. Phan, A. K. Raychaudhur, I. Das &amp; H. Srikanth</i>	9 (1)	Universality in the entropy change for the inverse magnetocaloric effect	<b>Phys. Rev. B</b> <b>87</b> , 134420 (2013)	3.7
25	<i>Kalipada Das,</i>		Giant enhancement of	<b>Appl. Phys. Lett.</b>	3.3



	<i>R. Rawat, B. Satpati &amp; I. Das</i>	<b>4 (3)</b>	magnetoresistance in core-shell ferromagnetic charge ordered nano structures	<b>103, 202406 (2013)</b>	
<b>26</b>	<i>Anis Biswas, Sayam Chandra, Tapas Samanta, M. H. Phan, I. Das &amp; H. Srikanth</i>	<b>6 (1)</b>	The universal behavior of inverse magnetocaloric effect in antiferromagnetic Materials	<b>J. Appl. Phys. 113, 17A902 (2013)</b>	<b>2.2</b>
<b>27</b>	<i>R. Rawat, P. Chaddah, P. Bag, Kalipada Das, &amp; I. Das</i>	<b>5 (2)</b>	The metal insulator transition in nanocrystalline $\text{Pr}_{0.67}\text{Ca}_{0.33}\text{MnO}_3$ : the correlation between supercooling and kinetic arrest	<b>J. Phys.: Condens. Matter 24, 416001 (2012)</b>	<b>2.3</b>

## Kalpataru Pradhan

Associate Prof. 'E', CMP Division (joining date: 03/12/2014)  
email-id: kalpataru.pradhan[AT]saha.ac.in



### Education:

B. Sc. Physics (Hons), Utkal University, Bhubaneswar (1998-2001)  
M. Sc. Physics (Specialization: Condensed Matter Physics), Bhubaneswar (2001-2003)  
Ph. D (Condensed Matter Physics), Harish-Chandra Research Institute, Allahabad (2003-2009)

### Research/Employment History

- 1) Associate Prof. 'E', *Dec 2014- to date*, Saha Institute of Nuclear Physics, Kolkata, India
- 2) Postdoctoral Fellow, *April 2014 – Nov 2014*, Computational Condensed Matter Physics, RIKEN, Wako, Japan.
- 3) Postdoctoral Fellow, *Nov 2011 - Dec 2013*, Institute of Physics, Augsburg University, Germany.
- 4) Postdoctoral Fellow, *Oct 2009 – Oct 2011*, Dept. Of Physics, VCU, Richmond, USA.

### Visiting Scientist positions:

- 1) Visiting Scientist, RIKEN, Wako, Japan (April 2016-March 2018).

### Publications (2012-2016):

- 1) “Magnetic reconstructions in B-site doped manganites”, [Kalpataru Pradhan](#), Journal of Applied Physics **119**, 033901 (2016).
- 2) “ $LiFe_2Cl_n$  ( $n=4-6$ ) clusters: Double-exchange mediated molecular magnets”, [Kalpataru Pradhan](#) and Puru Jena, Appl. Phys. Lett. **105**, 163112 (2014).
- 3) “Electronic and magnetic reconstructions in manganite superlattices”, [Kalpataru Pradhan](#) and Arno. P. Kampf, Phys. Rev. B **87**, 155152 (2013).
- 4) “Interfacial Magnetism in Manganite Superlattices”, [Kalpataru Pradhan](#) and Arno. P. Kampf, Phys. Rev. B **88**, 115136 (2013).
- 5) “Electronic and Magnetic Properties of Manganese and Iron Atoms decorated with  $BO_2$  Superhalogen”, Pratik Koirala, [Kalpataru Pradhan](#), Anil K. Kandalam, and P. Jena, J. Phys. Chem. A **117**, 1310 (2013).
- 6) “Evolution of superhalogen properties in  $PtCl_n$  clusters”, Jorly Joseph, [Kalpataru Pradhan](#), Puru Jena, Haopeng Wang, Yeon Jae Ko, Xinxing Zhang, and Kit Bowen, J. Chem. Phys. **136**, 194305 (2012).
- 7) “Doping induced magnetic transition in Mn-based molecular systems”, [Kalpataru Pradhan](#) and Puru Jena, Chem. Phys. Lett. **525-526**, **97** (2012).
- 8) “Functionalized Boranes for Hydrogen Storage”, Biswarup Pathak, [Kalpataru Pradhan](#), Tanveer Hussain, Rajeev Ahuja, Puru Jena, Chem. Phys. Chem **13**, 300 (2012).

### Three selected publications:

- 1) “Distinct Effects of Homogeneous Weak Disorder and Dilute Strong Scatterers on Phase Competition in the Manganites”, [Kalpataru Pradhan](#), Anamitra Mukherjee, and Pinaki Majumdar, Phys. Rev. Lett. **99**, 147206 (2007).
- 2) “Designer Magnetic Superatoms”, J. Ulises Reveles, P. A. Clayborne, Arthur C. Reber, S. N. Khanna, [Kalpataru Pradhan](#), Prasenjit Sen, and Mark R. Pederson, Nature Chemistry **1**, 310 (2009).
- 3) “Double exchange mediated ferromagnetic coupling between Co atoms in dicobalt complexes”, [Kalpataru Pradhan](#) and Puru Jena, Appl. Phys. Lett. **99**, 153105 (2011).

### Invited talks (Seminar/Conferences):

- 1) International Symposium on Clusters, Cluster Assemblies and Nanomaterials, IISER, Thiruvananthapuram (9<sup>th</sup>-12<sup>th</sup> March 2016). title: “Design of Molecular Ferromagnets”
- 2) National Seminar on “Current Trends in Physics”, Department of Physics, Utkal University, Bhubaneswar, Odisha (3<sup>rd</sup> January 2015). title: “Multiferroic Tunnel Junctions”

## Teaching:

- 1) Condensed Matter Physics (Dec 2015-July 2016)
- 2) Numerical Methods and Analysis (Aug-Nov 2015, Aug-Nov 2016)

## Ph.D. Students:

- 1) Sourav Chakraborty (joined: Aug 2016)

## Research Interest and future plan:

Transition metal oxides (TMOs) show a wide range of electrical and magnetic properties and bear promises of technological importance for the design of new functional materials. The physics is even much more richer at the interface of two TMOs. The central theme of our research is to find a correlation between the electronic and the magnetic properties at the interface. We also focus on the magnetic properties of atomic-clusters using density functional theory to design new tunable molecular-magnets.

We incorporated the long range Coulomb interaction into our model Hamiltonian (Hund's coupling + electron-phonon coupling) calculations, which controls the amount of electron transfer across the interface to explain the physics of **manganite heterostructures** [Phys. Rev. B 87, 155152 (2013), Phys. Rev. B 88, 155136 (2013)].

We have shown that the ferromagnetic ground states can be achieved via double-exchange interactions in di-nuclear transition metal complexes by altering the charge disproportionation between the transition metal atoms. [Chem. Phys. Lett. 525-526, 97 (2012), Appl. Phys. Lett. 105, 163112 (2014)]

**Oxide Heterostructures:** The goal is to theoretically understand the physics at the interface of transition metal oxides by using model Hamiltonian approach combined with material specific first-principles density functional theory calculations. We will mainly address the electronic and magnetic reconstructions at the interface between ferromagnetic (or antiferromagnetic) and ferroelectric materials in multiferroic tunnel junctions. Multiferroic tunnel junctions are potential candidates for future generation spintronics due to large tunneling electroresistance.

**Defect-induced magnetism in graphene:** Defect induced magnetism in graphene has attracted a great deal of interest during the last decade. Magnetic moments in graphene are believed to be formed due to over or under co-ordinated dangling bonds near the defect (the vacancies or the ad-atoms). We want to investigate the formation of magnetic moment(s) and possibility of long range magnetism in disordered graphene using model Hamiltonian (electron-electron interaction + long range Coulomb interaction + Hund's coupling) calculations.

**Controlling magnetism in nanostructures:** Density functional theory calculations will be used to analyze the magnetic properties of molecular magnets on a 2D substrate. We will focus di-nuclear transition-metal-based molecules on different 2D substrates e.g., graphene. Effect of external electric field will analyzed to design nano-materials with strong magneto-electric coupling.

## **Prabhat Mandal**

DOB: 01 November, 1959

### **Education:**

1992: Ph.D., University of Calcutta

1984: Post M. Sc. (Associateship)

1982: *M.Sc., (Physics) from the University of Calcutta*

### **Academic Positions:**

2014 – to date: Senior Professor 'H', Saha Institute of Nuclear Physics

2009-2014: Professor 'G', Saha Institute of Nuclear Physics

2006-2009: Professor 'F', Saha Institute of Nuclear Physics

2002-2006: Associate Professor 'E', Saha Institute of Nuclear Physics

1998-2002: Reader 'D', Saha Institute of Nuclear Physics

1996-1998: Lecturer 'C', Saha Institute of Nuclear Physics

1994-1996: Alexander von Humboldt Fellowship (Germany), University of Göttingen, Germany and Grenoble High Magnetic Field Lab, Grenoble, France,

1994-1994: Post-doctoral Fellow, Grenoble High Magnetic Field Lab, Grenoble, France, UNESCO Short-term Fellowship (UNESCO)

1993-1994: Post-doctoral Fellow, Grenoble High Magnetic Field Lab, Grenoble, France, C.I.E.S. Fellowship (French Govt. fellowship)

### **Awards/Honours/visiting Scientist:**

(i) Visiting Scientist, University of Augsburg, Germany for two months (1998); one month (2001); one month (2002); one month (2016).

(ii) Visiting Scientist, Max-Planck Institute for Solid State Research, Stuttgart, Germany for three months (2005).

(iii) Nominated scientist from India in the INSA-DFG Exchange Programme, Institute for Solid State Research (IFW), Dresden, Germany for three months (2005).

(iv) Nominated scientist from India in the INSA-DFG Exchange Programme, University of Augsburg,

Germany for five months (2000) and three months (2009).

(v) Received research award from the Third World Academy of Sciences and the Abdus Salam International Centre for Theoretical Physics, Trieste, Italy.

(vi) C.I.E.S. Fellowship (French Govt. fellowship); UNESCO Short-term Fellowship (UNESCO) and

Alexander von Humboldt Fellowship, Humboldt Foundation (Germany).

(vii) SINP Foundation Day Awards for high quality publications (2010, 2011).

**Publications:** In referred Journals: **150** (for 2012-16: **44**), Book Chapter: **2**  
[Physical Review B 43, APL 13, EPL 2, Physical Review Letter 1, PNAS 1, APL Material 1, Scientific Reports 3]

**PhD students since 2012 (Here, please give guide name, year of completion if degree awarded, also (if possible) present occupation of student etc.)**

**Guide: Prof. Prabhat Mandal**

Student: **Dr. Prosenjit Sarkar**; Present occupation: Faculty, Physics Department, Serampore College, Serampore, Hooghly, West Bengal, Degree awarded: 2013

Student: **Dr. Dilip Kumar Bhoi**; Present occupation: Post-doctoral fellow at Center for Novel States of Complex Materials Research and Institute of Applied Physics, Department of Physics and Astronomy, Seoul National University, Republic of Korea, Degree awarded: 2014

Student: **Dr. Arindam Midya**, Present occupation: Post-doctoral fellow at Physics Department, Faculty of Science, National University of Singapore, Singapore; Degree awarded: 2015

Student: **Dr. Nazir Khan**, Present occupation: Post-doctoral fellow at Center for Electronic Correlations and Magnetism, Augsburg University, Augsburg, Germany; Degree awarded: 2015

Student: **Dr. Moumita Nandi**, Present occupation: Degree awarded: 2017

Student: **Dr. Sourav Kundu**, Present occupation: Post-doctoral fellow S. N. Bose National Centre for Basic Sciences, Kolkata; Degree awarded: 2017

### **Important equipment and facility:**

1. Image Furnace for crystal growth (Crystal System, Japan) (Central Facility)
2. Physical Properties Measurement System (Quantum Design, USA) (Central Facility)
3. Cryogen Free Cooling System equipped with 9 T Superconducting Magnet
4. State-of-art home-made crystal growth facility by flux, chemical vapor transport techniques.
5. Several home-made facilities have been fabricated to measure different physical properties such as dielectric and ferroelectric, resistivity up to 800 K, thermoelectric power, angle dependent magneto-transport, etc.

### **Research highlight (last 5 years and future plan)**

#### **Magnetocaloric Effect:**

Energy efficient and environmentally friendly technology has received attention in order to combat the global warming phenomenon and energy crisis. Refrigeration based on the magnetocaloric effect (MCE) one such field of research because of its higher energy efficiency over the conventional refrigeration and it does not use ozone-depleting chlorofluorocarbon as a refrigerant. The main aim in this field is to search for new materials that exhibit a large MCE and are capable of operating at different temperature ranges, depending on the intended applications. Large MCE close to room temperature would be useful for domestic and several technological applications while large MCE in the low-temperature region is important for specific technological applications such as space science and liquefaction of hydrogen in fuel industry. In last few years, we are actively working in this field and have demonstrated that several magnetic materials showing huge MCE which are suitable for refrigeration in low temperature region. Examples:  $\text{EuTiO}_3$ ,  $\text{EuR}_2\text{O}_4$  (R=Ho, Dy),  $\text{RMnO}_3$  (R=Ho;Gd; Dy),  $\text{RCrO}_4$  (R=Ho,Gd,Lu), etc. We have also shown from our investigation on single crystals that highly anisotropic nature of MCE (rotating MCE) of some of the above materials has some technological advantage. Our works received considerable attention in the scientific community. In future, we would like focus our research to search new materials suitable for refrigeration at low temperature and around room temperature for technological application.

#### **Multifunctional and multiferroic materials:**

Since the discovery of multiferroic properties in hexagonal manganites, considerable research has been focused in this direction. In multiferroic compounds, two or more order parameters are coupled, as a result, there properties can be tuned easily by external perturbations. The magnetization can be controlled by the electric field and electric polarization can be tuned by magnetic field. As these materials have potential for several technological applications such as spintronic devices, information storage devices, spin valve, it is important to characterize them by investigating their physical properties. Based on our past experience and performance on manganite, we are also working in this field in collaboration with different groups in India.

#### **Strongly correlated electron system: Transition metal oxides:**

We have investigated the magneto-structural, magneto-transport, magnetic, thermal properties of several transition metal based strongly correlated electron systems in great details like  $\text{Na}_x\text{CoO}_2$ ,  $\text{La}_{1-x}\text{Sr}_x\text{CoO}_3$ ,  $\text{EuTi}_{1-x}\text{Nb}_x\text{O}_3$ , etc. Below, we have briefly discussed our contribution in this field.

### **Na<sub>x</sub>CoO<sub>2</sub> :**

We have investigated the magnetic and magnetotransport properties of high quality Na<sub>x</sub>CoO<sub>2</sub> single crystals in the heavily doped region ( $0.72 \leq x \leq 0.90$ ). Both the Hall coefficient ( $R_H$ ) and the susceptibility ( $\chi$ ) exhibit strong temperature dependence in the antiferromagnetic (AFM) as well as in the paramagnetic (PM) states. As the AFM ordering sets in, below  $T_N=21$  K,  $R_H$  decreases sharply with T down to  $\sim 10$  K and then increases rapidly. The temperature and field dependence of  $R_H$  indicates the emergence of a weak ferromagneticlike phase below 10 K. In the AFM state,  $R_H$  scales linearly with  $\chi$ . The observed T dependence of  $R_H$  in the PM state confirms the theoretical model proposed by Shastry for strongly correlated electrons in a triangular lattice.

### **La<sub>1-x</sub>Sr<sub>x</sub>CoO<sub>3</sub> :**

For understanding the magnetic and electronic properties and to draw a magnetic phase diagram for La<sub>1-x</sub>Sr<sub>x</sub>CoO<sub>3</sub>, we have studied different physical properties as a function of Sr concentration on very high quality single crystals of these materials.

The detailed analysis of the dc magnetization data in the vicinity of ferromagnetic transition, the scaling of the magnetization below  $T_C$  and susceptibility above  $T_C$ , suggests that the deduced values of critical exponents determined by different methods are consistent, unambiguous and intrinsic in nature. Furthermore, the obtained values of exponents suggest that for La<sub>1-x</sub>Sr<sub>x</sub>CoO<sub>3</sub> with  $x > 0.21$  the transition falls into the three-dimensional Heisenberg universality class of the near-neighbor interaction as proposed for double-exchange systems, whereas in the case of  $0.18 < x \leq 0.21$  the transition is characterized by mean-field-like values. The deviation of the critical exponents from 3D Heisenberg values toward mean-field ones is attributed to the presence of magnetoelectronic phase inhomogeneity in the  $x=0.21$  single crystal. The detailed analysis of the specific-heat data in the vicinity of  $T_C$  for the  $x=0.33$ ,  $0.25$ , and  $0.21$  samples also supports the phase separation scenario at around  $x=0.21$ . To the best of our knowledge, this type of analysis to detect the electronic phase separation in microscopic length scale has not been done before.

The nature of magnetic ground state for  $x < 0.18$  is not well established mainly due to the sample quality. We have made a detailed investigation of magnetic relaxation and memory effects in La<sub>0.9</sub>Sr<sub>0.1</sub>CoO<sub>3</sub> single crystal. The analysis of data below the freezing point  $T_f$  reveals the characteristics of spin-glass. The memory effect further establishes that the glassy magnetic state arises from the cooperative spin-spin interaction but not due to the independent relaxation of metastable phase clusters. The asymmetric response with respect to negative and positive temperature changes favors the hierarchical model of memory effects rather than the droplet model discussed in other works for different insulating and metallic Heisenberg spin glasses.

### **EuTi<sub>1-x</sub>Nb<sub>x</sub>O<sub>3</sub> :**

We have investigated the evolution of transport and magnetic properties in antiferromagnetic EuTiO<sub>3</sub> single crystals by introducing carrier via Nb substitution at Ti site. Conductivity is observed to increase dramatically with Nb doping and the system becomes metallic and ferromagnetic above 5% of Nb doping. The detailed analysis of temperature dependence of resistivity of EuTi<sub>1-x</sub>Nb<sub>x</sub>O<sub>3</sub> shows that several scattering mechanisms such as electron-magnon, electron-local moment and electron-electron are involved in charge transport. In the paramagnetic state,  $T^2$  and  $T^{3/2}$  temperature dependence of the resistivity have been observed which suggest an unusual crossover from a Fermi-liquid behavior to a non-Fermi-liquid behavior above 90 K. We have also observed resistivity upturn below 30 K which obeys  $\ln T$  behavior and suppresses with the application of magnetic field, indicating Kondo scattering of 4d<sup>1</sup> electron of Nb by localized 4f<sup>7</sup> moments of Eu<sup>2+</sup>.

### **Li-based chargeable battery for energy storage:**

In order to shade some light on the performance of Li-based battery, we have studied several physical properties of archetypal LiCo<sub>y</sub>Mn<sub>2-y</sub>O<sub>4</sub> and correlate the observed behavior with its

performance. The relation between electrochemical performance, activated-transport parameters, thermal expansion, and cooperativity of electron-phonon-interaction distortions has been discussed. The first order cooperative-normal-mode transition, detected through coefficient of thermal expansion, is found to disappear at a critical doping ( $y \sim 0.16$ ); interestingly, for  $y \sim 0.16$  the resistivity does not change much with doping and the electrochemical capacity becomes constant over repeated cycling. Our study reveals that the critical doping  $y \sim 0.16$  results in breakdown of the network of cooperative/coherent normal-mode distortions; this leads to vanishing of the first-order transition, establishment of hopping channels with lower resistance, and enhancing lithiation and delithiation of the battery, thereby minimizing electrochemical capacity fading.

### Topology protected electronic phases of matter:

In recent time, the topological concept in condensed matter electronic systems has received considerable attention. Over the last decade, the topological insulating phase of matter has emerged through the continuous evolution from two-dimensional quantum spin Hall state to three-dimensional (3D) topological insulators. This electronic phase of material has gaped bulk band like an ordinary insulator and protected conducting states on their edge or surface. 3D Dirac and Weyl type electronic materials are the most recently [Z. J. Wang et al. *PRB* (2012); Z. K. Liu et al. *Science* (2014); S. Y. Xu et al. *Science* (2015)] discovered quantum phase of matter, described as topological semimetal. Unlike topological insulator, bulk state in these materials is semimetal with linearly dispersing electronic band. The surface state is also distinct from spin-momentum locked closed Fermi circle of topological insulator. Due to the unique band topology, these materials show different exotic electronic properties of both fundamental and technological interest.

To study any physical property of a material, high quality single crystals are very important to decipher the role of several interactions. In our laboratory, we prepare high quality single crystal of these materials using different growth technique such as chemical vapor transport, flux method, etc. Our study is mainly concentrated on transport and magnetic properties, which have been established as powerful experimental tools to determine the technological importance and to understand the fundamental physics of these materials. Our recently published works are on 3D Dirac/Weyl semimetal candidates  $\text{Cd}_3\text{As}_2$ ,  $\text{ZrSiS}$  and  $\text{ZrTe}_5$ . We observe that the mobility of charge carriers in  $\text{Cd}_3\text{As}_2$ ,  $\text{ZrSiS}$ ,  $\text{ZrTe}_5$ ,  $\text{LaBi}$ , and  $\text{LaSbTe}$  is very high ( $\geq 10^4 \text{ cm}^2/\text{Vs}$ ), and these materials show giant and anisotropic transverse magneto resistance ( $\sim 10^3$  to  $10^5$  % at 2 K and 9 tesla), which indicates the possibility for technological application as fast electronic device and magnetic field sensor. A pronounced surface dominated metallic charge transport over the insulation bulk has been reported by our group in three dimensional topological insulator  $\text{Bi}_{1.5}\text{Sb}_{0.5}\text{Te}_{1.7}\text{Se}_{1.3}$ , which is the necessary criterion for the utilization of spin helical metallic surface state in spintronic application.

Beside the technological impact, we are interested in fundamental physics of these materials too. We have probed the Fermi surface geometry of  $\text{Cd}_3\text{As}_2$ ,  $\text{ZrSiS}$  and  $\text{LaBi}$  by analyzing Shubnikov–de Haas oscillations in magneto-transport and De Haas–van Alphen oscillations in magnetization measurements. All the physical parameters associated to Fermi surface (such as effective mass of charge carrier, Fermi velocity, Fermi wave vector, scattering time, etc.) have been determined to understand the charge transport mechanism in these materials. In addition to the nature and geometry of the Fermi surfaces, we have also analyzed the scattering mechanism and different unusual physical phenomenon of this type of materials. A wide tunability of the charge-scattering mechanism has been realized by varying the strength of the magnetic field and the carrier density via indium doping in  $\text{Cd}_3\text{As}_2$ . With the increase in magnetic field, the scattering time crosses over from being nearly energy independent to a regime of linear dependence. On the other hand, the scattering time enters into the inverse energy-dependent regime and the Fermi surface strongly modifies with 2% In doping at Cd atom site. The Wiedemann-Franz law (which states that the ratio of electronic thermal conductivity to the product of temperature and electrical conductivity is a



universal constant in a conventional metal) has been found to violate drastically under application of magnetic field in  $\text{Cd}_3\text{As}_2$ .

The relativistic theory of charged chiral fermions in three spatial dimensions holds the so-called chiral anomaly- non-conservation of chiral charge induced by external gauge fields with non-trivial topology, known as Adler-Bell-Jackiw (ABJ) anomaly. Theory predicts that, condensed matter systems having 3D Dirac/Weyl type excitation in their electronic band structure, may be a suitable place to observe ABJ anomaly. Measuring resistivity under electric field parallel to magnetic field (longitudinal) configuration, one can find enhanced magneto conductance, i.e., negative magnetoresistance due to ABJ anomaly. In our magneto-transport experiment on  $\text{ZrSiS}$  and  $\text{ZrTe}_5$ , we have been able to observe the chiral anomaly induced negative longitudinal magnetoresistance. The non-trivial  $\pi$  Berry's phase acquired by the electron due to cyclotron orbit around the Dirac node has also been obtained in  $\text{Cd}_3\text{As}_2$ ,  $\text{ZrSiS}$  and  $\text{LaBi}$ . These above mentioned findings have established the three dimensional linear dispersion of bulk electronic band in these materials.

Employing magnetization measurements, we have been able to discover the spin helical Dirac cone band of topological surface states in bulk linear dispersing material  $\text{ZrTe}_5$ . This allows one to conclude that  $\text{ZrTe}_5$  is a novel quantum phase of matter, which hosts both the topological Dirac fermions on the surface and three-dimensional Dirac cone band spectrum in the bulk, unlike earlier reported 3D topological insulators. Subsequently, our finding was supported by ARPES study. Later on, using the same technique, we have confirmed the existence of this type surface Dirac cone state in  $\text{Bi}_{1.5}\text{Sb}_{0.5}\text{Te}_{1.7}\text{Se}_{1.3}$  and  $\text{LaBi}$ . As is a relatively new field, we are interested to continue our research along this direction in order to search new materials which are suitable for fundamental interest as well as technological applications.

### Single Crystal Growth Facility:

High quality single crystals are essential for fundamental research in condensed matter physics. There are several techniques to grow single crystals. Often we need large size high quality single crystals for specific studies. Image furnace provides an opportunity to grow large single crystals of several materials with relatively high melting point. As no crucible is used in this technique, one can avoid the possibility of contamination. With the existing image furnace, we have grown high quality single crystals of several rare-earth and transition metal based oxide compounds. This system allows us to use different kinds of gaseous atmosphere (oxygen, nitrogen, air, argon, etc.) at ambient pressure as well high pressure. The materials having melting point below 2000 °C can be grown using the present image furnace.

We have also set-up state-of-art crystal growth facility for low melting point material in a sealed atmosphere using flux melting, chemical vapor transport, etc. We also have designed indigenously the method to separate the flux which does not dissolve in water or any liquid. These fluxes are removed by centrifuge method keeping the temperature of the mixture slightly above the melting point of the flux. Single crystals of several topological materials viz.  $\text{Cd}_3\text{As}_2$ ,  $\text{ZrSiS}$ ,  $\text{ZrTe}_5$ ,  $\text{NbSb}_2$ ,  $\text{LaBi}$ ,  $\text{LaSbTe}$ ,  $\text{Bi}_{1.5}\text{Sb}_{0.5}\text{Te}_{1.7}\text{Se}_{1.3}$ , etc. have been grown using these techniques.

## Individual CV (only from 2012 onwards)

### List of Publications in referred Journals 2012-2017

1. Magnetoelectronic phase separation in  $\text{La}_{1-x}\text{Sr}_x\text{CoO}_3$  single crystals: Evidence from critical behavior

N. Khan, **P. Mandal**, K. Mydeen, D. Prabhakaran  
Phys. Rev. B **85** 214419 (2012)

2. Anomalous thermal expansion of  $\text{Sb}_2\text{Te}_3$  topological insulator

- P. Dutta, D. Bhoi, A. Midya, N. Khan, **P. Mandal**, S. S. Samatham, V. Ganesan  
*Appl. Phys. Lett.* **100**, 251912 (2012)
3. Scaling of non-Ohmic conduction in strongly correlated systems  
D. Talukdar, U.N. Nandi, A. Poddar, **P. Mandal**, K.K. Bardhan  
*Phys. Rev. B* **86**, 165104 (2012)
  4. Hall effect in the metallic antiferromagnet  $\text{Na}_x\text{CoO}_2$  ( $0.72 \leq x \leq 0.90$ )  
**P. Mandal**, P Choudhury  
*Phys. Rev. B* **86**, 094423 (2012)
  5. **Giant magnetocaloric effect in magnetically frustrated  $\text{EuHo}_2\text{O}_4$  and  $\text{EuDy}_2\text{O}_4$  compounds**  
A. Midya, N. Khan, D. Bhoi and P. Mandal  
*Appl. Phys. Lett.* **101**, 132415 (2012)
  6. Colossal piezoresistance effect in  $\text{Sm}_{0.55}(\text{Sr}_{0.5}\text{Ca}_{0.5})_{0.45}\text{MnO}_3$  single crystal  
D.M. Radheep, P. Sarkar, S. Arumugam, **P. Mandal**  
*Appl. Phys. Lett.* **102**, 092406 (2013)
  7. Electric field driven destabilization of the insulating state in nominally pure  $\text{LaMnO}_3$   
R. Nath, A.K. Raychaudhuri, Y.M. Mukovskii, P. Mondal, D. Bhattacharya, **P. Mandal**  
*J. Phys.: Cond. Matter* **25**, 155605 (2013)
  8. Critical exponents and irreversibility lines of  $\text{La}_{0.9}\text{Sr}_{0.1}\text{CoO}_3$  single crystal  
N. Khan, A. Midya, **P. Mandal**, D. Prabhakaran  
*Journal of Applied Physics* **113**, 183909 (2013)
  9. Vortex dynamics and second magnetization peak in  $\text{PrFeAsO}_{0.6}\text{F}_{0.12}$  superconductor  
D. Bhoi, P. Mandal, P. Choudhury  
*Journal of Applied Physics* **113**, 183902 (2013)
  10. Formation of nanosize griffiths-like clusters in solid solution of ferromagnetic manganite and cobaltite  
D. Bhoi, N Khan, A. Midya, M Nandi, A. Hassen, P. Choudhury, **P. Mandal**  
*The Journal of Physical Chemistry C* **117**, 16658 (2013)
  11. 3d-4f spin interaction induced giant magnetocaloric effect in zircon-type  $\text{DyCrO}_4$  and  $\text{HoCrO}_4$  compounds  
A. Midya, N. Khan, D. Bhoi, **P. Mandal**  
*Appl. Phys. Lett.* **103**, 092402 (2013)
  12. Large magnetocapacitance in electronic ferroelectric manganite systems  
U. Chowdhury, S. Goswami, D. Bhattacharya, A. Midya, **P. Mandal**, P. Das, Y. M Mukovskii  
*Journal of Applied Physics* **114**, 194104 (2013)
  13. Temperature-dependent structural property and power factor of n type thermoelectric  $\text{Bi}_{0.9}\text{Sb}_{0.1}$  and  $\text{Bi}_{0.86}\text{Sb}_{0.14}$  alloys  
K. Malik, D. Das, S. Bandyopadhyay, **P. Mandal**, A.K. Deb, V. Srihari, A. Banerjee  
*Appl. Phys. Lett.* **103**, 242108 (2013)

14. Field-Induced Spin-Structural Transition and Giant Magnetostriction in Ising Chain  $\alpha$ -CoV<sub>2</sub>O<sub>6</sub>  
M. Nandi, N. Khan, D. Bhoi, A. Midya, **P. Mandal**  
The Journal of Physical Chemistry C 118, 1668 (2014)
15. Memory effects and magnetic relaxation in single-crystalline La<sub>0.9</sub>Sr<sub>0.1</sub>CoO<sub>3</sub>  
N. Khan, **P. Mandal**, D. Prabhakaran  
Phys. Rev. B 90, 024421 (2014)
16. Giant magnetocaloric effect in antiferromagnetic DyVO<sub>4</sub> compound  
  
A. Midya, N. Khan, D. Bhoi, **P. Mandal**  
  
Physica B: Condensed Matter 448, 43 (2014)
17. Critical end point of the first-order ferromagnetic transition in a Sm<sub>0.55</sub>(Sr<sub>0.5</sub>Ca<sub>0.5</sub>)<sub>0.45</sub>MnO<sub>3</sub> single crystal  
D.M. Radheep, P. Sarkar, S. Arumugam, R. Suryanarayanan, **P. Mandal**  
Journal of Magnetism and Magnetic Materials 365, 51 (2014)
18. 3d-4f spin interaction and field-induced metamagnetism in RCrO<sub>4</sub> (R= Ho, Gd, Lu) compounds  
A. Midya, N. Khan, D. Bhoi, **P. Mandal**  
Journal of Applied Physics 115, 17E114 (2014)
19. Effect of pressure on the magnetic and superconducting transitions of GdFe<sub>1-x</sub>Co<sub>x</sub>AsO (x= 0, 0.1, 1) compounds  
G.K. Selvan, D. Bhoi, S. Arumugam, A. Midya, **P. Mandal**  
Superconductor Science and Technology 28, 015009 (2014)
20. Comparative Study of the Layered Perovskites Pr<sub>1-x</sub>A<sub>1+x</sub>CoO<sub>4</sub>(A= Sr, Ca)  
A. Hassen, A. Krimmel, **P. Mandal**  
Journal of the American Ceramic Society 97, 3609 (2014)
21. Giant magnetocaloric effect in ferromagnetic superconductor RuSr<sub>2</sub>GdCu<sub>2</sub>O<sub>8</sub>  
A. Midya, **P. Mandal**  
Journal of Applied Physics 116, 223905 (2014)
22. Probing the Fermi surface of three-dimensional Dirac semimetal Cd<sub>3</sub>As<sub>2</sub> through the de Haas– van Alphen technique  
A. Pariari, P. Dutta, **P. Mandal**  
Phys. Rev. B 91, 155139 (2015)
23. Spin dynamics and frequency dependence of magnetic damping study in soft ferromagnetic FeTaC film with a stripe domain structure  
B. Samantaray, A.K. Singh, A. Perumal, R. Ranganathan, **P. Mandal**  
AIP Advances 5, 067157 (2015)
24. Perpendicular standing spin wave and magnetic anisotropic study on amorphous FeTaC films  
B. Samantaray, A. Singh, C. Banerjee, A. Barman, A. Perumal, **P. Mandal**  
IEEE Transactions on Magnetics 52, 2003104 (2016)

25. Field-induced ferromagnetism due to magneto-striction in 1-D helical chains  
B.K. Shaw, M. Das, A. Bhattacharyya, B.N. Ghosh, S. Roy, **P. Mandal**, K. Rissanen,  
S. Chattopadhyay, S. K. Saha  
RSC Advances 6, 22980 (2016)
26. Giant magnetothermal conductivity and magnetostriction effect in the charge ordered  
 $\text{Nd}_{0.8}\text{Na}_{0.2}\text{MnO}_3$  compound  
B. Samantaray, N. Khan, A. Midya, S. Ravi, **P. Mandal**  
Europhysics Letters 113, 17003 (2016)
27. Giant low-field magnetocaloric effect in single-crystalline  $\text{EuTi}_{0.85}\text{Nb}_{0.15}\text{O}_3$   
S. Roy, N. Khan, **P. Mandal**  
APL Materials 4, 026102 (2016)
28. Field induced metamagnetic transitions in quasi-one-dimensional Ising spin chain  $\text{CoV}_2\text{O}_6$   
M. Nandi, **P. Mandal**  
Journal of Magnetism and Magnetic Materials 400, 121 (2016)
29. Low Gilbert damping and in-plane magnetic anisotropy in Ni–Mn–Sn thin film with high  
L21 order  
R. Modak, B. Samantaray, **P. Mandal**, A. Srinivasan  
Applied Physics A 122, 1 (2016)
30. Large adiabatic temperature and magnetic entropy changes in  $\text{EuTiO}_3$   
A. Midya, **P. Mandal**, K. Rubi, R. Chen, J.S. Wang, R. Mahendiran, G. Lorusso, M. Evangelisti  
Phys. Rev. B 93, 094422 (2016)
31. Magnetoelectric coupling and exchange bias effects in multiferroic  $\text{NdCrO}_3$   
A. Indra, K. Dey, A. Midya, **P. Mandal**, O. Gutowski, U. Rütt, S. Majumdar, S. Giri  
Journal of Physics: Condensed Matter 28, 166005 (2016)
32. Magnetic and magnetocaloric properties of quasi-one-dimensional Ising spin chain  $\text{CoV}_2\text{O}_6$   
M Nandi, **P Mandal**  
Journal of Applied Physics 119, 133904 (2016)
33. Determination of intrinsic ferroelectric polarization in lossy improper ferroelectric systems  
U. Chowdhury, S. Goswami, D. Bhattacharya, A. Midya and **P. Mandal**  
Appl. Phys. Lett. 109, 092902 (2016)
34. Tuning the scattering mechanism in the three-dimensional Dirac semimetal  $\text{Cd}_3\text{As}_2$   
A Pariari, N. Khan, R. Singha, B. Satpati, **P Mandal**  
Phys. Rev. B 94, 165139 (2016)
35. Coexistence of topological Dirac fermions in the surface and three-dimensional Dirac cone  
state in the bulk of  $\text{ZrTe}_5$  single crystal  
A. Pariari, **P. Mandal**  
Scientific Reports 7, 40327 (2017)

36. Large nonsaturating magnetoresistance and signature of non-degenerate Dirac nodes in ZrSiS  
R. Singha, A. Pariari, B. Satpati, **P. Mandal**  
Proceedings of the National Academy of Sciences 114, 2468 (2017)
37. Thickness dependent structural, magnetic and magneto-dynamic properties of Mn rich Ni-Mn-Sn films  
R. Modak, B. Samantaray, **P. Mandal**, A. Srinivasan  
Journal of Alloys and Compounds 692, 529 (2017)
38. Continuously varying critical exponents beyond weak universality  
N. Khan, P. Sarkar, A. Midya, **P. Mandal**, P. Mohanty  
Scientific Reports 7, 45004 (2017)
39. Geometrically frustrated GdInO<sub>3</sub>: An exotic system to study negative thermal expansion and spin-lattice coupling  
B. Paul, S. Chatterjee, A. Roy, A. Midya, P. Mandal, V. Grover, A. K. Tyagi  
Phys. Rev. B **95**, 054103 (2017)
40. Magnetoelectric memory in reentrant frozen state and considerable ferroelectricity in the Multiferroic spin-chain compound Sm<sub>2</sub>BaNiO<sub>5</sub>  
A Indra, K Dey, S Majumdar, I Sarkar, S Francoual, RP Giri, N Khan, ...  
Phys. Rev. B 95, 094402 (2017)
41. Jahn Teller Effect in LiMn<sub>2</sub>O<sub>4</sub>: influence on charge ordering, magnetoresistance and battery performance  
K.R. Rao, H. Xia, P. Mandal, A.K. Arof  
Physical Chemistry Chemical Physics **19**, 2073 (2017)
42. Correlation between battery material performance and cooperative electron-phonon interaction in LiCo<sub>y</sub>Mn<sub>2-y</sub>O<sub>4</sub>  
K. R. Ragavendran, P. Mandal, S. Yarlagadda  
Appl. Phys. Lett. **110**, 143901 (2017);
43. Magnetic ordering induced ferroelectricity in α-Cu<sub>2</sub>V<sub>2</sub>O<sub>7</sub> studied through non-magnetic Zn doping  
B. Chattopadhyay, M. A. Ahmed, S. Bandyopadhyay, R. Singha, P. Mandal  
Journal of Applied Physics 121, 094103 (2017)
44. Prominent metallic surface conduction and the singular magnetic response of topological Dirac fermion in three-dimensional topological insulator Bi<sub>1.5</sub>Sb<sub>0.5</sub>Te<sub>1.7</sub>Se<sub>1.3</sub>  
P. Dutta, A. Pariari, **P. Mandal**  
Scientific Reports Scientific Reports 7, 4883 (2017)

## Seminar given in National/International Conference/Workshop

1. **P. Mandal** (invited speaker)  
Worldwide Universities Network (WUN) International Conference on Spintronics, Sydney, Australia, July 23-25, 2012
2. **P. Mandal**  
International conference on Magnetism and Magnetic Materials, Denver, CO, United States, Nov 04-08, 2013
3. **P. Mandal** (invited speaker)  
9<sup>th</sup> India-Singapore joint Symposium, National University of Singapore, February 24-26, 2016.
4. **P. Mandal** (invited speaker)  
Recent Trends in Condensed Matter Physics: Experiment and Theory, IACS, Kolkata, March 3-4, 2017
5. **P. Mandal** (invited speaker)  
Indo-French Workshop on Pressure Effects on Strongly Correlated Materials, Bharathidasan University, Tiruchirappalli, January 9-12, 2017
6. **P. Mandal** (invited speaker)  
National Workshop on Condensed Matter Physics, IIT Kharagpur, February 03 - 05, 2017.

## Awards/Honours/visiting Scientist

- (i) Received C.I.E.S. Post-Doctoral Fellowship (French Govt. fellowship) at Grenoble High Magnetic Field Lab (GHMFL), Grenoble, France, 1993-94.
- (ii) Received UNESCO Short-term Fellowship (UNESCO) at Grenoble High Magnetic Field Lab (GHMFL), Grenoble, France, 1994-94.
- (iii) Received Alexander von Humboldt Fellowship (Germany) to pursue research at University of Göttingen, Germany and Grenoble High Magnetic Field Lab (GHMFL), Grenoble, France, 1994-96.
- (iv) Visiting Scientist, University of Augsburg, Germany for two months (1998); one month (2001); one month (2002); one month (2016).
- (v) Visiting Scientist in Max-Planck Institute for Solid State Research, Stuttgart, Germany for three months (2005).
- (vi) Nominated scientist from India in the INSA-DFG Exchange Programme, Institute for Solid State Research (IFW), Dresden, Germany for three months (2005).

## Reviewer of the following journals of international repute:

Physical Review Letters, [Physical Review B](#), Applied Physics Letter, [Journal of Appl. Phys.](#), [Physica B](#), [Physica C](#), [Physica Scripta](#), [European Journal of Physics B](#), [Physics Letter A](#), [Solid State Communication](#), [Indian Journal of Pure & Applied Physics](#), [Indian Journal of Physics \(A&B\)](#), [Phase Transitions](#), [Materials Science & Engineering B](#), [Applied Surface Science](#), [Nature Communication](#), [Scientific Reports](#), [Journal of Physics and Chemistry of Solids](#), [Journal of Physical Chemistry C](#), [Journal of alloys and compounds](#), [New Journal of Physics](#), [Journal of Materials Chemistry C](#), [Journal of Physics: Condensed Matter](#), [Journal of Magnetism and Magnetic Materials](#), [Materials Research Bulletin](#), [RAC Advances](#), [Superconducting Science & Technology](#).

### **Other Academic Responsibility:**

Being a Joint Coordinator of Post. M. Sc (Expt. Physics stream) teaching, I am very much involved in designing and conducting post M. Sc course, teaching, organizing meetings, admission test, interview and selection and other necessary and related academic activities.

**Teaching:** I also take classes on condensed matter for post M. Sc students who are supposed to join for Ph. D after completing the one year course work.

## **Prof. Pradeep Kumar Mohanty**

CMP Division, Saha Institute of Nuclear Physics, HBNI  
1/AF Bidhan Nagar, Kolkata 700064, INDIA  
E-mail : [pk.mohanty@saha.ac.in](mailto:pk.mohanty@saha.ac.in)



### **Basic Information:**

**1. Present position :** Prof. G (since 1st Jan, 2013)  
ID : 1050 Basic : Rs. 51,510 Grade Pay: Rs. 8,900

### **2. PhD completed since 2012**

- 1) Urna Basu (Feb'13), SISSA, Trieste, Italy
- 2) Debarshee Bagchi (Nov'14), CBPF, Rio, Brazil
- 3) Mahashweta Basu (Apr'15), Univ. Maryland, USA
- 4) Sourish Bandyopadhyay (Jul'15), working as Met. Scientist, India
- 5) Bijoy Daga (submitted)

**3. Important equipment and facility:** None

**4. Research highlight :** *mentioned in the CV*

**5. Individual CV :** *Attached.*

## **Curriculum Vitae (2012-2016)**

### **I. CAREER PROFILE**

- Ph.D. in August 2000 from Harischandra Research Institute, Allahabad, India
- Postdoctoral Fellow at Tata Institute of Fundamental Research, Mumbai, India (Aug'00- Sept'02)
- Feinberg Fellow at Weizmann Institute of Science, Israel (Sept'02- Sept'04)
- Visiting Scientist at MaxPlanck Institute(PKS), Dresden, Germany (Sept'04-Oct'05)
- Associate Professor E in CMP Division at Saha Institute of Nuclear Physics (Nov'05- Aug'08)
- Professor F at CMP Division, Saha Institute of Nuclear Physics (Sept'08 - Dec'2012 )
- Professor G at TCMP Division, Saha Institute of Nuclear Physics (Jan'2013 - )
- Visiting Professor at MaxPlanck Institute(PKS), Dresden, Germany (Aug'14-Aug'15)

### **II. Research Highlights**

I am deeply involved in understanding the universality class of self-organized criticality (SOC). In a recent work [PRL 2012] we show, for the first time, that the critical fluctuations in these systems are unusual, violate the law of large numbers -relaxation to such low-fluctuating-states takes very long, which might be the reason why earlier studies have been contradictory to each other. We propose a special initial states to avoid these ill effects and show that criticality here belong to the well known Directed Percolation universality class. This work has a great impact in the theory of self-organized criticality and in non-equilibrium phase transitions. Soon after the work it was discovered [PRL 2015] that a low-fluctuating-critical-state, namely hyperuniformity, is a generic feature of all absorbing phase transitions (like percolation, wetting, surface pinning etc.). At



the same time, Le-Dussal et. al. [PRL 2015] claimed, by mapping the field theory of stochastic models of SOC to that of surface growth in disordered media (quenched Edward Wilkinson models), that directed percolation (DP) may not be the correct universality class. A rigorous numerical study by the nominee along with Dhar and Grassberger [PRE, 2016] also indicated that the field theoretic arguments were right and firmly establish, for the first time, that universality other than DP is possible in SOC ;certain additional perturbations (or symmetry) could be holding some models in DP class. I will be working towards establishing the exact nature of such perturbations.

Existence of equilibrium-like state functions are not guaranteed for current carrying systems - can we build a thermodynamic structure for such non-equilibrium systems ? Recently we show [PRL 2014] that for conserved non-equilibrium systems with short-range correlation, one can always write a free-energy function which is additive. The prove relies on the fact that the subsystem mass distribution of such systems can be derived from knowing the functional form of fluctuations in terms of the conserved density. Linear mass-redistribution dynamics, often used for modeling nonequilibrium mass transport models, lead to a quadratic functional dependence - this explains `why locally measured quantities (say mass) in conserved systems often show Gamma-like distributions ?' We also find a sufficient condition on contact-dynamics [PRE, 2015] that ensures zeroth law for two non-equilibrium systems in contact.

*How mutation make big changes ?* From the preferential interaction partners of the wild type and mutant proteins, HTT and TP53 (whose mutation causes Huntington's disease and Cancer, respectively) we construct the protein interaction network and identify protein modules which does specific biological processes [PlosONE 2013]. This differential approach reveals the plausible loss and gain of functions which may occur due to mutation.

Spinal cord injury (SCI) is one of the leading causes of morbidity. Right after the insult a plethora of molecular changes sets in leading the patients to a secondary stage of complete, or incomplete injury. With the help of doctors and biologists we try to assimilate the enriched proteins in the cerebrospinal fluid of the patients, and then identify the respective functions which are altered. We propose that proteins Zinc alpha 2 and haptoglobin could hasten recovery [PlosONE 2014]. We have also shown [Mol. Cell. Bio. Chem, 2016] that ApoA1, a well known player in reverse cholesterol transport is increasingly abundant at a later time point in the secondary phase of traumatic spinal cord injury. In neuroblastoma injury model, we observe that an initial lag in scratch wound closure was followed by rapid healing in the ApoA1 treatment group.

### III. OTHER INFORMATION

- **Articles in last 5 years (2012-2016)**

I have co-authored 21 articles in last 5 years in various international journals. This includes 2 PRL, 3 EPL,PRE, 2 PlosONE, 1 PRB and 3 JSTAT.

- **Teaching**

Adv. Stat. Mech. (2016, 2015, 2013)

- **PhD produced**

- 1) Urna Basu (Feb'13), SISSA, Italy
- 2) Debarshee Bagchi (Nov'14), CBPF, Rio, Brazil
- 3) Mahashweta Basu (Apr'15), Univ. Maryland, USA
- 4) Sourish Bandyopadhyay (Jul'15), Met. Scientist, Pune, India

5) Bijoy Daga (submitted)

• **Referee and Editor :**

I have been a regular referee of PRL, PRE, JSTAT, J. Stat. Phys, JPhys. A, Physica A and Pramana. I am associate editor of Frontiers in Physics and guest edited Physica A 384(1).

• **Planning, organization**

- Member, Indo-French CEFIPRA prog.(2012-14)
- Convenor, KOLSYSBIO, Kolkata, Jan'13
- Organizer STATPHYS-Kolkata VIII, Dec'14

• **Talks in Conferences(2013-15):**

- Seminar Series in Complex Systems, 14-24 Mar, 2016, IOPB, Bhubaneswar, India
- Indian Statistical Physics Community meeting, 12-14 Feb, 2016, Bangalore, India
- Criticality in Biology: A Critical Assessment, 07-17 Apr, 2015, MPIPKS, Dresden, Germany
- Random Walks and Nonlinear Dynamics in the Life of Cells, 18-22 May 2015, MPIPKS, Dresden, Germany.
- Dynamics of Coupled Oscillators: 40 Years of the Kuramoto Model, 27-31 Jul 2015, MPIPKS, Dresden, Germany.
- Percolation and the Glass Transition, 19-23 Oct, 2014, Tel Aviv University, Israel
- Indian Statistical Physics Community meeting, Feb 2014, Bangalore, India
- Science Academies Refresher Course in Statistical Physics, May 2013, Kanhangad, Kerala, India

• **Visits and Talks**

LPTMS, Orsay and CEA Saclay (Dec'15, Sep'13); Wurzburg Univ.(Sept'14); Tel Aviv Univ (Oct'14); ICTS and RRI; Bangalore (Mar'13, Feb'16); TIFR, Mumbai (Sep'12, Oct'16); IMSc, NCBS and JNCASR (Jan'12); IOP, Bhubaneswar (Sep'11, Mar'16); Weizmann Institute (Oct'14)

## Publications(2012-2016)

\* *Biophysics related works are marked blue.*

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### 2016

[1] The Oslo model, hyperuniformity, and the quenched Edwards-Wilkinson model, P. Grassberger, D Dhar and PKM, Phys.Rev. E 94, 042314 (2016).

[2] Phase coexistence and spatial correlations in reconstituting k-mer models, A. K. Chatterjee, B. Daga and PKM, Phys. Rev.E 94, 012121 (2016).

[3] Continuously Varying Critical Exponents Beyond Weak Universality, N. Khan, P. Sarkar, A. Midya, P. Mandal, and PKM, arXiv:1604.07688 (to appear in Sc. Reports).

[4] Multi-critical absorbing phase transition in a class of exactly solvable models, A Chatterjee, and PKM, Phys. Rev. E 94, 062141 (2016).

[5] ApoA1 promotes growth in injured neuroblastoma M. B. Sengupta, S. Saha, PKM, K.K. Mukhopadhyay, and D. Mukhopadhyay, Mol. Cell. Bio. Chem. 1-11 (2016)

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### 2015

[6] Additivity property and emergence of power laws in nonequilibrium steady states A Das, S Chatterjee, P Pradhan, PKM, Phys. Rev. E 92, 052107 (2015).

[7] Cluster-factorized steady states in finite-range processes, A Chatterjee, P Pradhan, PKM, *Phys. Rev. E* 92, 032103 (2015).

[8] Zeroth law and nonequilibrium thermodynamics for steady states in contact, S Chatterjee, P Pradhan, PKM, *Phys. Rev. E* 91, 062136 (2015).

[9] Phase separation transition of reconstituting k-mers in one dimension, B Daga, PKM, *JSTAT* P04004 (2015).

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**2014**

[10] Self-organised criticality in stochastic sandpiles: Connection to directed percolation, U Basu and PKM, *Euro. Phys. Lett.* 108, 60002 (2014).

[11] A microscopic model of ballistic-diffusive crossover, D Bagchi and PKM, *JSTAT*, P11025 (2014).

[12] CSF Proteomics of Secondary Phase Spinal Cord Injury in Human Subjects: Perturbed Molecular Pathways Post Injury, MB Sengupta, M Basu, S Iswarari, KK Mukhopadhyay, KP Sardar, B Acharyya, PKM, and D Mukhopadhyay, *PLoS ONE* 9, e110885 (2014).

[13] Universality splitting in distribution of number of miRNA co-targets, M Basu, NP Bhattacharyya, PKM, *Syst. Synth. Bio.* 8, 21 (2014).

[14] Gammalike mass distributions and mass fluctuations in conserved-mass transport processes S Chatterjee, P Pradhan, and PKM, *Phys. Rev. Lett.* 112, 030601 (2014).

[15] Distribution of microRNA co-targets exhibit universality across a wide class of species, M Basu, NP Bhattacharyya, and PKM, *Euro. Phys. Lett.* 105, 28007(2014).

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**2013**

[16] Comparison of Modules of Wild Type and Mutant Huntingtin and TP53 Protein Interaction Networks: Implications in Biological Processes and Functions, M. Basu, N. P. Bhattacharyya, and PKM, *PLoS ONE* 8(5): e64838 (2013)

[17] Absorbing phase transition in energy exchange models, U. Basu, Ma-hashweta Basu, and PKM, *Eur. Phys. J. B* 86, 236(2013).

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**2012**

[18] Fixed-Energy Sandpiles Belong Generically to Directed Percolation, M. Basu, U. Basu, S. Bondyopadhyay, PKM, and H. Hinrichsen, *Phys. Rev. Lett.* 109, 015702 (2012)

[19] Thermally driven classical Heisenberg model in one dimension, D. Bagchi, and PKM, *Phys. Rev. B* 86, 214302 (2012)

[20] Restricted Exclusion Processes without Particle Conservation Flows to Directed Percolation, U. Basu, and PKM, *Euro.Phys. Lett.* 99, 66002 (2012)

[21] Conserved mass models with stickiness and chipping, S. Bondyopadhyay, and PKM, *J. Stat. Mech.* (2012) P07019

## Sudhakar Yarlagadda

Present position, Div. : Head & Sr. Professor, CMP Division

### Phd students and Postdoc guidance:

1) My student, Dr. Sanjoy Datta, (who received his PhD in 2009); postdoc at HRI from 2009 to 2012; postdoc at LPMMC, Grenoble (France) from Aug./2012 to Aug./2014; Asst. Prof. at NIT Rourkela since Aug./2014.

2) Our (Prof. P. B. Littlewood's and my) student Sahinur Reja (who was a Saha-Cavendish Fellow) got his PhD from Cambridge Univ. In Nov./2013; he was a postdoc at IFW, Dresden (Germany) in Prof. Jeroen van den Brink's group till March/2016; he is currently a postdoc at Indiana Univ. in Prof. Herb Fertig's group.

3) My student Amit Dey successfully defended his thesis in May/2016; he is currently a postdoc in Ben-Gurion University, Israel.

4) My student M. Q. Lone (Asst. Professor at Univ. of Kashmir) is trying to finish his PhD; we have written a few papers together.

5) I am currently guiding the PhD work of the following students:

- i) Ravindra Pankaj
- ii) Amrita Ghosh
- iii) Sanjukta Paul

6) I had Dr. Satyaki Kar working with me as a postdoc (2013 to 2015); he is currently a postdoc at IACS, Kolkata.

7) I (along with Prof. P. Mandal) guided a postdoc Dr. K. Ragavendran (2014 to 2016); joined recently as an Asst. Prof. at the University (Kalasalingam Academy of Education and Research), near Madurai, Tamilnadu.

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**Important equipment and facility:** Not Applicable.

### Research Highlights (2012-2017):

#### Important contributions made to fundamental knowledge or original developments

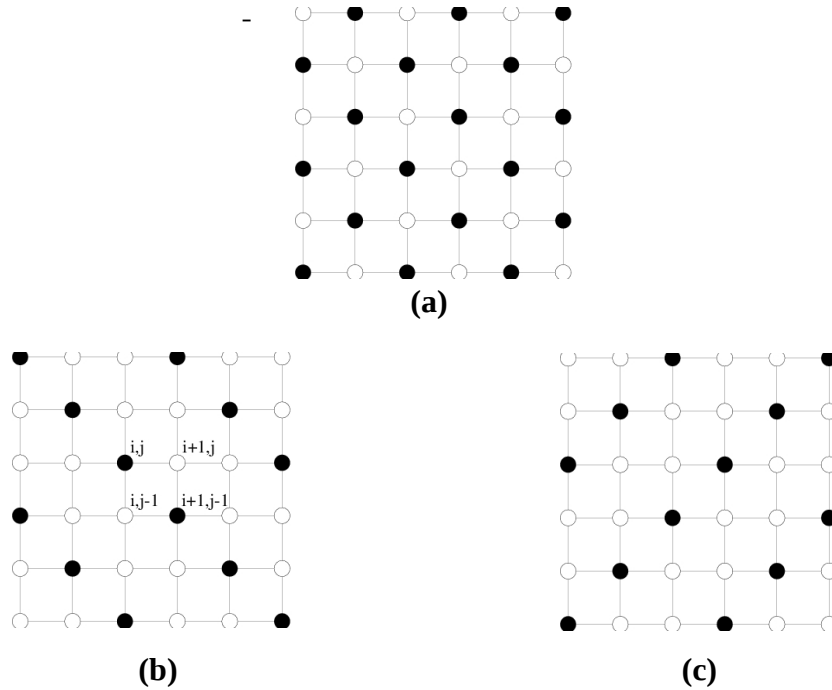
The main ideas in the following works were mine.

#### A) Supersolidity in Hard-Core-Boson (HCB) systems

Understanding the microscopic mechanism of coexisting long-range orders (such as lattice supersolidity) in naturally occurring and artificially designed strongly correlated systems has been and will continue to be an area of immense interest. While phenomenological pictures exist to explain lattice-supersolidity, a microscopic theory that elucidates the homogeneous coexistence is yet to be formulated.

We study lattice systems of HCBs strongly-coupled to optical phonons. *Devising a strong-weak duality treatment, we map strong-coupling problems (in the original frame of reference) to weak-coupling problems (in the dual frame of reference) with the small parameter being the inverse of that in the original frame of reference.* Our duality treatment is potentially employable in various fields of physics dealing with strong coupling between fermions/HCBs and massive bosonic excitations (such as optical phonons, plasmons, etc.). In the dual frame of reference, effective Hamiltonians are derived using perturbation theory. The effective Hamiltonians (for HCBs strongly-coupled to optical phonons) belong to the class of extended boson Hubbard models of the type  $\mathbf{t}_1\text{-}\mathbf{t}_2\text{-}\dots\text{-}\mathbf{t}_m\text{-}\mathbf{V}_1\text{-}\mathbf{V}_2\text{-}\dots\text{-}\mathbf{V}_n$  [involving hoppings  $\mathbf{t}_1, \mathbf{t}_2, \mathbf{t}_3$ , etc. and interactions  $\mathbf{V}_1, \mathbf{V}_2, \mathbf{V}_3$ , etc. of ranges nearest neighbor (NN), next-nearest neighbor (NNN), next-to-next-nearest neighbor (NNNN), etc.]. Unlike many lattice models of the extended boson Hubbard type, the parameters (i.e., hopping term, strength of HCB-phonon coupling, and phonon frequency) in our  $\mathbf{t}_1\text{-}\mathbf{t}_2\text{-}\dots\text{-}\mathbf{t}_m\text{-}\mathbf{V}_1\text{-}\mathbf{V}_2\text{-}\dots\text{-}\mathbf{V}_n$  model either can be determined from band-structure calculations or can be obtained from experiments. It is important to point out that our derivations [see Sanjoy Datta, Arnab Das, and Sudhakar Yarlagadda, Phys. Rev. B, **71** 235118 (2005) and later works] also correct the oversight in the effective Hamiltonian (obtained from a different approach for the one-dimensional Holstein Model) reported in the well-cited work of Jorge E. Hirsch and Eduardo Fradkin, Phys. Rev. B **27**, 4302 (1983).

The minimum model for realizing a checkerboard supersolid (**cSS**) is shown to be the  $\mathbf{t}_2\text{-}\mathbf{V}_1$  model. On the other hand,  $\mathbf{t}_1\text{-}\mathbf{V}_1\text{-}\mathbf{V}_2\text{-}\mathbf{V}_3$  model is demonstrated to be the minimum model for obtaining a rare diagonal striped supersolid (**dsSS**). The mechanism governing the existence of a supersolid phase away from commensurate fillings, on unfrustrated system (such as the square lattice), is that interstitials or vacancies can move without a cost in the potential energy; however, importantly, particles on the crystal lattice also take part in the superflow.



**FIG. 1. Different types of CDWs:** (a) checkerboard solid (**cS**) at half-filling with  $S(\mathbf{Q})$  peaking at  $\mathbf{Q}=(\pi,\pi)$ ; (b) diagonal striped solid (**dsS**) indicated by peak in  $S(\mathbf{Q})$  at  $\mathbf{Q}=(2\pi/3,2\pi/3)$ ; and (c) **dsS** characterized by ordering wavevector  $\mathbf{Q}=(2\pi/3,4\pi/3)$ .

### [A.1\) Checkerboard-supersolidity in a two-dimensional Bose-Holstein model](#)

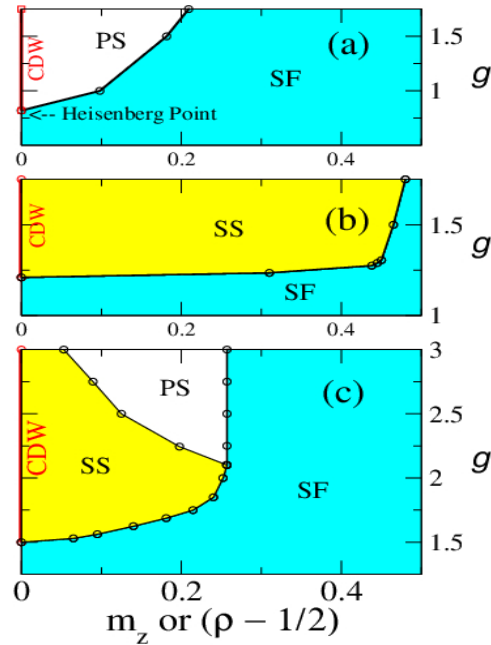
Satyaki Kar and Sudhakar Yarlagadda, *Annals of Physics* **375**, 322 (2016).

Here we study the cooperation/competition of the superfluid and charge-density-wave (CDW) orders in a two-dimensional Bose-Holstein model where HCBs are coupled locally to optical phonons. In the parameter regimes of strong HCB-phonon coupling and nonadiabaticity, we find a novel mechanism for lattice-supersolidity (namely, sizeable same-sublattice tunneling in presence of large nearest-neighbor repulsion) in the system. The ground state phase diagram is obtained using Quantum Monte Carlo simulation involving stochastic-series-expansion technique. At densities not far from half filling and in the parameter regime where the double-hopping terms are non-negligible (negligible) compared to the nearest-neighbor hopping, we get checkerboard-supersolidity (phase separation) with CDW being characterized by ordering wavevector  $\mathbf{Q} = (\pi, \pi)$ .

The following effective  $\mathbf{t}_1$ - $\mathbf{t}_2$ - $\mathbf{t}_3$ - $\mathbf{V}_1$  Hamiltonian for the HCB particles on a 2D square lattice is obtained:

$$H_e = -g^2 \omega_0 \sum_j n_j - t_1 \sum_{j,\delta} b_j^\dagger b_{j+\delta} - t_2 \sum_{j,\delta'} b_j^\dagger b_{j+\delta'} - t_3 \sum_{j,\delta''} b_j^\dagger b_{j+\delta''} - V_1/2 \sum_{j,\delta} n_j (1 - n_{j+\delta}) \quad (1)$$

where  $\delta'$  and  $\delta''$  denote next-nearest-neighbor (NNN) and next-to-next-nearest neighbor (NNNN) sites respectively;  $t_1 = t \exp(-g^2)$ ,  $t_2 = 2t^2 \exp(-g^2)/(g^2 \omega_0)$ ,  $t_3 = t_2/2$ , and  $V_1 \sim t^2/(g^2 \omega_0)$



**FIG. 2. Quantum phase diagrams at various magnetizations  $m_z$  (or fillings  $\rho$ ) and HCB-phonon coupling  $g$  when adiabaticity  $t/\omega_0 = 1.0$ .** The calculations are for a 16X16 lattice and for our BH system [using Eq. (1)] by (a) considering interaction and only nearest-neighbor hopping, i.e.,  $t_2 = t_3 = 0$ ; (b) setting  $t_1 = 0$ , i.e., considering interaction and only NNN and NNNN hoppings; and (c) including interaction and all the hoppings. Here PS, SS, and SF refer to Phase Separation, Supersolid, and Superfluid.

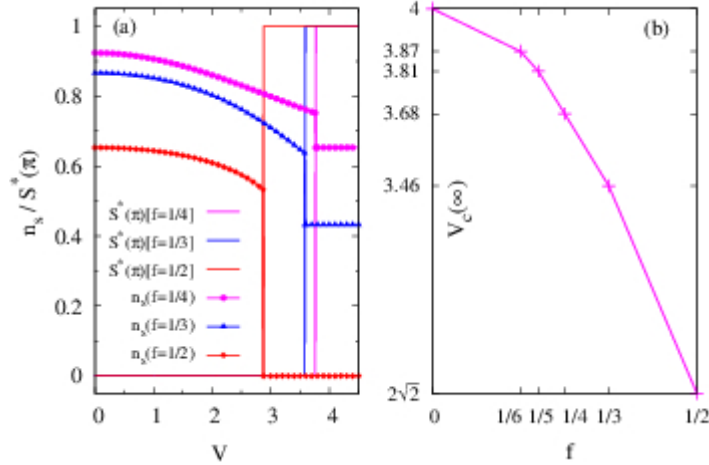
## A.2) An analysis of the $t_2$ - $V$ model

Amrita Ghosh and Sudhakar Yarlagadda, Phys. Rev. B **90**, 045140 (2014).

Some time ago, we derived the effective Hamiltonian for the cooperative electron-phonon interaction (EPI) quantum systems in one-dimension [R. Pankaj and S. Yarlagadda, PRB **86**, 035453 (2012)]; it has been demonstrated analytically that introducing cooperative effects in the strong EPI limit changes the dominant transport mechanism from one of nearest-neighbor (NN) hopping to that of next-nearest-neighbor (NNN) hopping. Additional NN particle repulsion (due to incompatibility of distortions produced by cooperative EPI effects) leads to the  $t_1$ - $t_2$ - $V_1$  model as the effective model. Recently (after us) T. Mishra, R. V. Pai, and Subroto Mukerjee [PRA **89**, 013615 (2014)] studied the  $t_1$ - $t_2$ - $V_1$  model.

We study a novel model (i.e., the  $t_2$ - $V_1$  model involving next-nearest-neighbor hopping and nearest-neighbor repulsion) in one dimension that generically depicts the dominant transport mechanism in cooperative strong electron-phonon interaction systems. Using analytic and numerical approaches, hard-core bosons are shown to typically undergo a striking discontinuous transition from a superfluid to a supersolid. Topological inequivalence of rings with even and odd number of sites is manifested through observable differences (in structure factor peaks) at the transition. Connections are also identified between the  $t_2$ - $V_1$  model and other topologically interesting models.

The above work (on the  $t_2$ - $V_1$  model) has been used/extended by X. Huo, Y.-Y. Cui, D. Wang, and J.-P. Lv, Phys. Rev. A **95**, 023613 (2017); T. Bilitewski and N. R. Cooper Phys. Rev. A **94**, 023630 (2016); R. W. Chhajlany, P. R. Grzybowski, J. Stasinska, M. Lewenstein, and O. Dutta Phys. Rev. Lett. **116**, 225303 (2016).

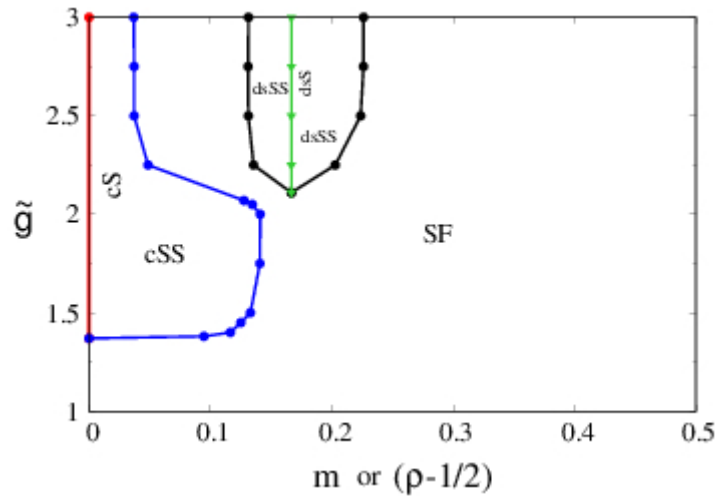


**FIG. 3.** (a) Plots of rescaled structure factor  $S^*(\pi)$  and superfluid fraction  $n_s$  at various filling factors  $f$  obtained using modified Lanczos technique. The calculations were at  $f = 1/2, 1/4$  with system size  $N_s = 16$  and at  $f = 1/3$  with  $N_s = 12$ . At a critical repulsion there is a striking discontinuous transition; while  $S^*(\pi)$  jumps from its minimum to maximum, there is a significant drop in  $n_s$ . (b) Plot of  $V_c(\infty)$  (critical repulsion for an infinite system) obtained from Green's function analysis for half-filled ( $f = 1/2$ ) and two-HCB systems ( $f \rightarrow 0$ ) and from finite size scaling at various other fillings  $f$ .

### [A.3\) Study of long-range orders of hard-core bosons coupled to cooperative normal modes in two-dimensional lattices.](#)

Amrita Ghosh and Sudhakar Yarlagadda, arXiv:1610.01447

We study the possible manifestations of long-range orders, including lattice-supersolid phases with differently broken symmetry, in a two-dimensional square lattice system of HCBs coupled to archetypal cooperative/coherent normal-mode distortions such as those in perovskites. At strong HCB-phonon coupling, using a duality transformation, we obtain an effective Hamiltonian  $\mathbf{t}_1\text{-}\mathbf{t}_2\text{-}\mathbf{t}_3\text{-}\mathbf{V}_1\text{-}\mathbf{V}_2\text{-}\mathbf{V}_3$  involving nearest-neighbor, next-nearest-neighbor, and next-to-next-nearest-neighbor hoppings and repulsions. Using stochastic series expansion quantum Monte Carlo, we construct the phase diagram of the system. As coupling strength is increased, we find that the system undergoes a first-order quantum phase transition from a superfluid to a checkerboard solid at half filling and from a superfluid to a diagonal striped solid [with crystalline ordering wavevector  $\mathbf{Q} = (2\pi/3, 2\pi/3)$  or  $(2\pi/3, 4\pi/3)$ ] at one-third filling without showing any evidence of supersolidity. On tuning the system away from these commensurate fillings, checkerboard supersolid is generated near half filling whereas a rare diagonal striped supersolid is realized near one-third filling. Interestingly, there is an asymmetry in the extent of supersolidity about one-third filling. We identify the  $\mathbf{t}_1\text{-}\mathbf{V}_1\text{-}\mathbf{V}_2\text{-}\mathbf{V}_3$  model as the minimum model for obtaining a diagonal striped supersolid on a square lattice. Within our framework, we also provide an explanation for the observed checkerboard and diagonal-stripe formations in  $\text{La}_{2-x}\text{Sr}_x\text{NiO}_4$  at  $x=1/2$  and  $x=1/3$ .



**FIG. 4. Phase diagram in terms of magnetization (or filling-fraction  $\rho$  and HCB-phonon coupling for HCBs on a 18X18 lattice with adiabaticity  $t/\omega_0 = 1.0$ . cS represents checkerboard solid with cSS being the corresponding supersolid; dsS stands for diagonal striped solid with dsSS being the related supersolid. Plots represent averaged results from simulations employing three different random number seeds.**

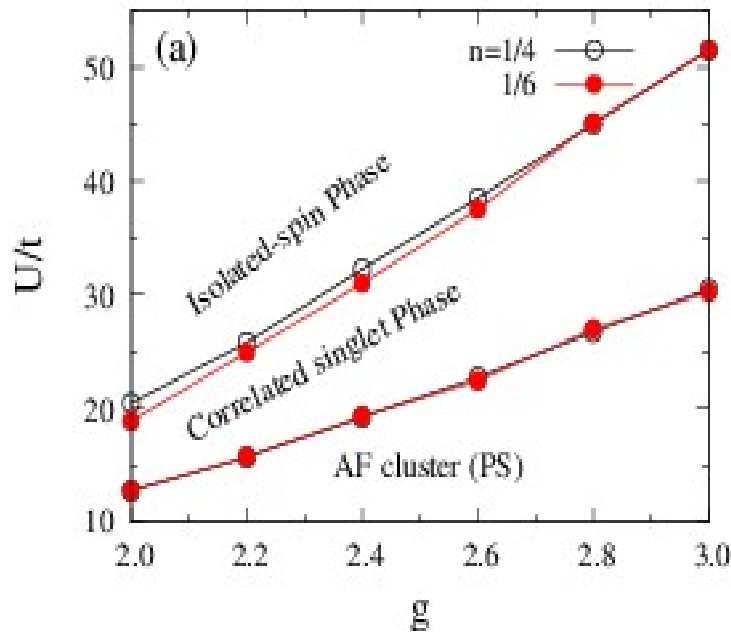
### [A.4\) Correlated singlet phase in the one-dimensional Hubbard-Holstein model](#)

Sahinur Reja, Sudhakar Yarlagadda, Peter B. Littlewood, Phys. Rev. B **86**, 045110 (2012).

A wealth of materials show evidence of strong electron-phonon (e-ph) interactions besides the ubiquitous electron-electron (e-e) interactions. For instance, transition metal oxides such as cuprates and manganites and molecular solids such as fullerides indicate strong e-ph coupling  $g$ . The interplay of e-e and e-ph interactions in these correlated systems leads to coexistence of or competition between various phases such as superconductivity, CDW, etc.



We derived an effective Hamiltonian for the one-dimensional Hubbard-Holstein model (using our duality treatment) and obtained the phase diagram at various fillings. As e-e interaction is increased, the system transits from an antiferromagnetic cluster to a correlated nearest-neighbor singlet phase (see figure below). We have analyzed the correlated nearest-neighbor singlet phase predicted by the effective Hamiltonian of the Hubbard-Holstein model by essentially mapping the Hamiltonian onto the well-understood one-dimensional  $\mathbf{t}_1\text{-}\mathbf{V}_1$  model with large repulsion. Because the physics is dictated by the  $\mathbf{t}_1\text{-}\mathbf{V}_1$  model, we find that CDW and superfluidity occur mutually exclusively with CDW resulting only at  $\mathbf{n} = 1/3$  while superfluidity manifests itself at all other fillings. We also show that the BEC occupation number  $\mathbf{n}_0$  for our model scales similarly to the  $\mathbf{n}_0$  of a HCB-tight-binding model; additionally, we demonstrate numerically (using our new world-line QMC method and a modified Lanczos algorithm), at  $\mathbf{n} = 1/3$ , that the  $\mathbf{n}_0$  for our model is smaller than the  $\mathbf{n}_0$  for a HCB tight binding model.



**FIG. 5.** Plots obtained using modified Lanczos in a twelve-site system for  $\mathbf{t}/\omega_0 = 1.0$ . Phase diagram (at various dimensionless e-e interactions  $U/t$  and e-ph couplings  $g$ ) depicts that the phase transition lines are close for both densities  $\mathbf{n} = 1/4$  and  $\mathbf{n} = 1/6$ .

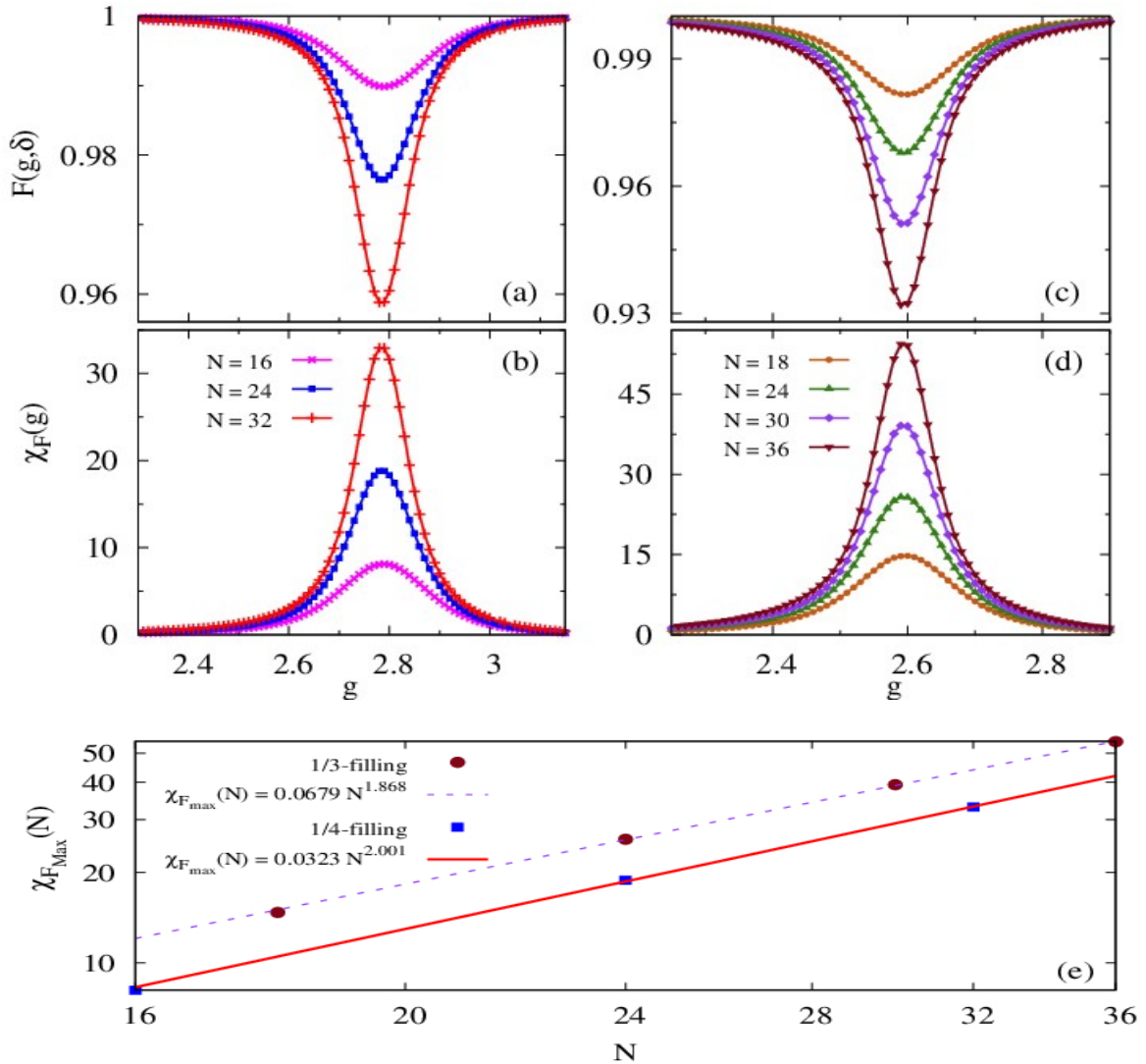
## **B) Using strong-weak duality to analyze systems with strong cooperative electron-phonon interaction**

The last few decades have witnessed numerous studies to fathom the tapestry of exotic phenomena (such as long-range orderings) and interesting functionalities (such as colossal magnetoresistance, multiferroicity, superconductivity, etc.) in bulk transition metal oxides (such as the manganites, cuprates, etc.) and their interfaces. To model the emergent ordering and functionality in these complex metal oxides (and guide material synthesis), one needs, as building blocks, effective Hamiltonians for various interactions. Except for the cooperative electron-phonon interaction (EPI), effective Hamiltonians, that reasonably mimic the physics, have been derived for all other interactions. For instance, double exchange model approximates infinite Hund's coupling,

Gutzwiller approximation or dynamical mean-field theory model Hubbard on-site Coulombic interaction, superexchange describes localized spin interaction at strong on-site repulsion, etc. Many oxides such as cuprates, manganites, and bismuthates indicate cooperative strong EPI.

### B.1) Study of cooperative breathing-mode in molecular chains

Ravindra Pankaj and Sudhakar Yarlagadda, Phys. Rev. B **86**, 035453 (2012)



**FIG. 6.** Ground state fidelity (GSF)  $F(g, \delta)$  in the CBM model at adiabaticity  $t/\omega_0 = 0.1$  and  $\delta = 0.05$  for (a) 1/4 filling and (c) 1/3 filling. Fidelity susceptibility (FS)  $\chi_F(g)$  for (b) 1/4 filling and (d) 1/3 filling correspond to the GSF plots in (a) and (c). (e) Plot of the peak values of FS  $\chi_{F, \max}(N)$  versus  $N$ , on a logarithmic scale, at 1/4 filling and 1/3 filling and the corresponding power-law fits.

Many oxides that have the formula  $ABO_3$  assume a perovskite structure where two adjacent  $BO_6$  octahedra share an oxygen which leads to cooperative octahedral distortions. Understanding the cooperative electron-phonon phenomena in systems such as the bismuthates, the cuprates, and the manganites is still an open question. Using a controlled analytic nonperturbative treatment (involving a duality transformation) that accounts for the quantum nature of the phonons, we derive a model that generically describes the cooperative breathing-mode (CBM) at strong electron-phonon interaction in one-band one-dimensional systems [PRB **86**, 035453]. The effective model involves a next-nearest-neighbor hopping (that dominates over the nearest-neighbor hopping at strong coupling) and a nearest-neighbor repulsion that is significantly enhanced due to incompatibility of neighboring dilations/compressions. At non-half-filling, upon tuning the electron-phonon coupling, the system undergoes a period-doubling second-order quantum phase transition from a Luttinger liquid to a conducting commensurate charge-density-wave state: a phenomenon absent in both the Holstein model and the  $t_1-V_1$  model. Using fidelity to study the nature of the quantum phase transition, we find that the fidelity susceptibility shows a superextensive power law divergence as well as a remarkable scaling behavior; both together establish a second-order transition (see figures above).

## **[B.2\) Charge and orbital order due to cooperative Jahn-Teller effect in manganite chains.](#)** [Ravindra Pankaj, Sudhakar Yarlagadda, arXiv:1608.06055](#)

We derive an effective Hamiltonian that takes into account the quantum nature of phonons and models cooperative Jahn-Teller effect in the adiabatic regime and at strong electron-phonon coupling in one dimension. Our approach involves mapping a strong-coupling problem to a weak-coupling one by using a duality transformation. Subsequently, a sixth-order perturbation theory is employed in the polaronic frame of reference where the small parameter is inversely (directly) proportional to the coupling (adiabaticity). We study charge and orbital order in ferromagnetic manganite chains and address the pronounced electron-hole asymmetry in the observed phase diagram. In particular, at strong coupling, we offer an explanation for the observed density dependence of the wavevector of charge modulation, i.e., wavevector is proportional to (independent of) electron density on the electron-doped (hole-doped) side of the phase diagram of manganites. We also provide a picture for the charge and orbital order at special fillings  $1/2$ ,  $1/3$ ,  $1/4$ , and  $1/5$ ; while focusing on the ordering controversy at fillings  $1/3$  and  $1/4$ , we find that Wigner-crystal arrangement is preferred over bi-stripe order.

## **[C\) Oxide devices as replacement for semiconductor devices](#)**

Although semiconductors are the most widely used functional materials for electronic applications so far, nevertheless, semiconductor devices have some limitations: i) the characteristic length scales are sizeable so that further scaling down the existing system size is quite difficult; and ii) only the charge and spin degrees of freedom are utilized. On the other hand, owing to significantly smaller extent of the wavefunction, transition metal oxides can meet the miniaturization demands much better than semiconductors. Furthermore, oxides offer a vastly richer physics involving diverse spin, charge, lattice, and orbital correlations. Low-dimensional oxides present new opportunities for devices where these diverse correlations can be optimized by engineering many-body interactions, fields, geometries, disorder, strain, etc. Therefore, oxides may be viewed as one of the best candidates to replace semiconductors in future electronic devices.

### [C.1.1\) Study of decoherence in models for hard-core bosons coupled to optical phonons](#)

A. Dey, M. Q. Lone, and S. Yarlagadda, *Phys. Rev. B* **92**, 094302 (2015).

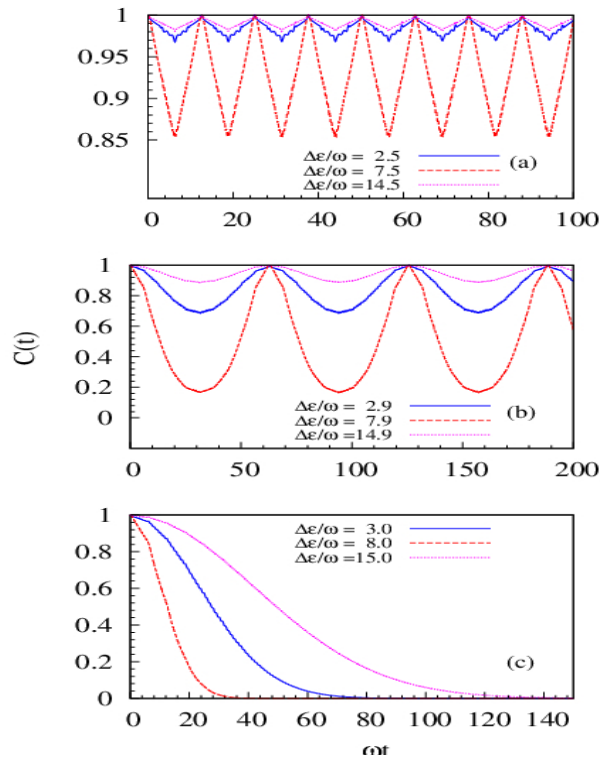
### [C.1.2\) Polaron dynamics and decoherence in an interacting two-spin system coupled to an optical-phonon environment](#), Amit Dey and S. Yarlagadda, *Phys. Rev. B* **89**, 064311 (2014).

Understanding coherent dynamics of excitons, spins, or hard-core bosons (HCBs) has tremendous scientific and technological implications for quantum computation. Here, we study decay of excited-state population and decoherence in a two-site HCB model with site-dependent strong potentials and subject to non-Markovian dynamics. The model is investigated in the regimes of antiadiabaticity and strong HCB-phonon coupling with each site providing a different local optical phonon environment; furthermore, the HCB system is taken to be initially uncorrelated with the environment in the polaronic frame of reference. We show clearly that the degree of decoherence and decay of excited state are enhanced by the proximity of the site-energy difference to the eigenenergy of phonons and are most pronounced when the site-energy difference is at resonance with twice the polaronic energy; additionally, the decoherence and the decay effects are reduced when the strength of HCB-phonon coupling is increased.

The model Hamiltonian is given by

$$H = \epsilon_1(n_1 - 1/2) + \epsilon_2(n_2 - 1/2) - J_{\perp}/2 (b_1^{\dagger} b_2 + b_2^{\dagger} b_1) + J_{\parallel} (n_1 - 1/2) (n_2 - 1/2) + g\omega \sum_{i=1,2} (n_i - 1/2)(a_i + a_i^{\dagger}) + \omega \sum_{i=1,2} (a_i^{\dagger} a_i) \quad (2)$$

where  $\epsilon_1$  and  $\epsilon_2$  are the site energies,  $J_{\perp}/2$  ( $>0$ ) is the hopping, and  $J_{\parallel}$  ( $>0$ ) is the repulsion strength between HCBs on the adjacent sites.



**FIG. 7.** Time ( $\omega t$ ) dependence of  $C(t)$  for  $J_{\perp} / \omega = 0.5$ ,  $g=2.0$ , and when (a)  $\Delta\epsilon/\omega = 2.5$ , 7.5, and 14.5; (b)  $\Delta\epsilon/\omega = 2.9$ , 7.9, and 14.9; and (c)  $\Delta\epsilon/\omega = 3.0$ , 8.0, and 15.0.

In the two-site HCB model, the dynamics of population as well as the coherence are important for understanding physical systems such as a double quantum dot (DQD) acting as a qubit for quantum computation. An oxide- (i.e., manganite-) based DQD, with appropriate detuning, can serve as a charge qubit with very small decoherence compared to a semiconductor DQD; furthermore, it can also meet the demands of miniaturization as its size can also be much smaller than a semiconductor DQD.

### [C.2\) Temperature dependence of long coherence times of oxide charge qubits.](#)

[A. Dey, S. Yarlagadda, arXiv:1610.01866](#)

$K_B T / \omega_u$	$\Delta \epsilon / \omega_u$	0.0	0.2	0.5	0.8
0.01		>100 s	>100 s	>100 s	>100 s
0.15		50 ps	24 $\mu$ s	> 0.1 s	83 ns
0.50		1 ps	47 ps	0.75 $\mu$ s	10 ps

TABLE. I. Coherence times at various values of scaled thermal energy  $K_B T / \omega_u$  and detuning energy  $\Delta \epsilon / \omega_u$  when optical phonon energy  $\omega_u = 0.05$  eV.

The ability to maintain coherence and control in a qubit is a major requirement for quantum computation. We show theoretically that long coherence times can be achieved above boiling point of liquid helium in charge qubits of oxide double quantum dots. Detuning the dots to a fraction of the optical phonon energy, increasing the electron-phonon coupling, reducing the adiabaticity, or decreasing the temperature enhances the coherence time. We consider a system that is initially decoupled from the phonon bath in the polaronic frame of reference and solve the non-Markovian quantum master equation; we find that the system decoheres after a long time, despite the fact that no energy is exchanged with the bath.

### [C.3\) Giant magnetoelectric effect in pure manganite-manganite heterostructures.](#)

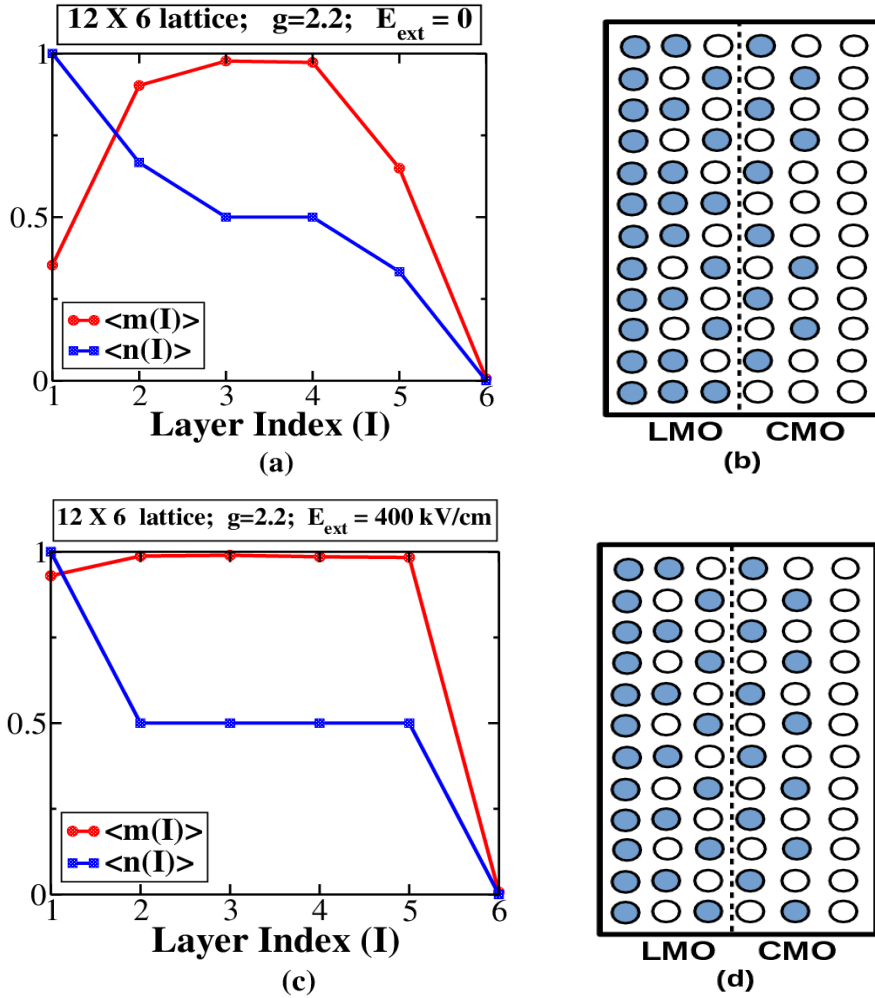
[Sanjukta Paul, Ravindra Pankaj, Sudhakar Yarlagadda, Pinaki Majumdar, Peter B. Littlewood, arXiv:1702.06302](#)

Obtaining strong magnetoelectric couplings in bulk materials and heterostructures is an ongoing challenge. We demonstrate that manganite heterostructures of the form

$$\text{(Insulator)/(LaMnO}_3\text{)}_n\text{/Interface/(CaMnO}_3\text{)}_n\text{(Insulator)}$$

show strong multiferroicity in magnetic manganites where ferroelectric polarization is realized by

charges leaking from  $\text{LaMnO}_3$  to  $\text{CaMnO}_3$  due to repulsion. Here, an effective nearest-neighbor electron-electron (electron-hole) repulsion (attraction) is generated by cooperative electron-phonon interaction. Double exchange, when a particle virtually hops to its unoccupied neighboring site and back, produces magnetic polarons that polarize antiferromagnetic regions. Thus a striking giant magnetoelectric effect ensues when an external electrical field enhances the electron leakage across the interface.



**FIG. 8.** In a symmetric 12X6 lattice, for coupling  $g = 2.2$ , (a) at zero electric field, layer-averaged charge density  $\langle n(I) \rangle$  and layer-averaged magnetization  $\langle m(I) \rangle$  of  $t_{2g}$  spins normalized to unity; (b) at  $E_{\text{ext}} = 0$ , ground state configuration; (c) at strong external electric field  $E_{\text{ext}} = 400 \text{ V/cm}$ , layer-averaged charge density  $\langle n(I) \rangle$  and layer-averaged magnetization  $\langle m(I) \rangle$  of  $t_{2g}$  spins normalized to unity; and (d) at  $E_{\text{ext}} = 400 \text{ kV/cm}$ , charge configuration in the ground state.

#### [D\) Correlation between battery material performance and cooperative electron-phonon interaction in \$\text{LiCo}\_y\text{Mn}\_{2-y}\text{O}\_4\$](#)

K. Ragavendran, P. Mandal, and S. Yarlagadda, *Appl. Phys. Lett.* **110**, 143901 (2017).

So far designing new battery materials has been based on intuition and chemical concepts. However, it is highly essential to couple these efforts with basic physics (experimental and theoretical) investigations so that better batteries can be designed. Despite the fact that battery materials show striking similarities with the perovskite manganites and sodium cobaltate,

problems in battery materials are hardly addressed by the physics community. The present work establishes the much-needed correlation between battery performance and basic physics pertaining to battery material (such as  $\text{LiCo}_y\text{Mn}_{2-y}\text{O}_4$ ). It is believed that the present study will provide a new insight into designing Li-ion battery cathodes and stimulate further research activity, along similar directions, among the physicists.

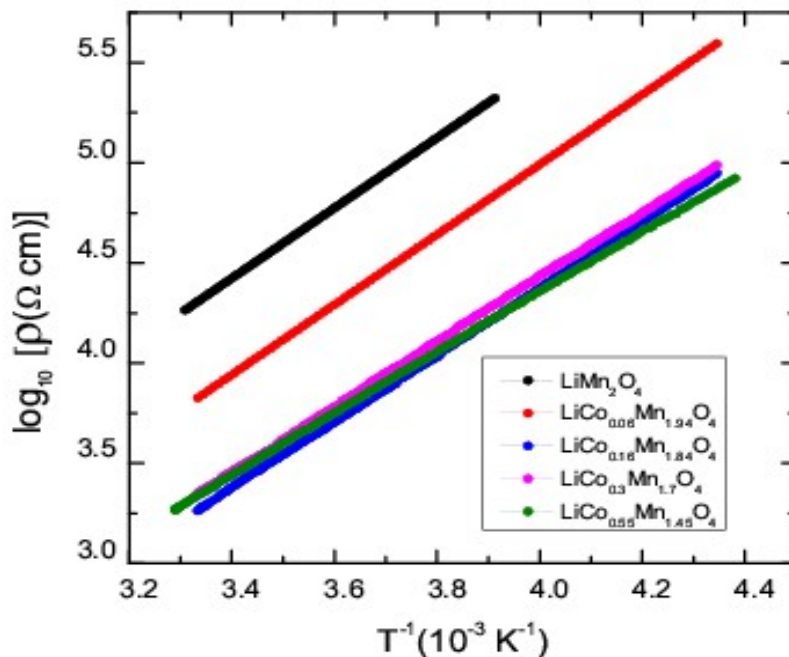
The relation between electrochemical performance, activated-transport parameters, thermal expansion, and cooperativity of electron-phonon-interaction distortions in  $\text{LiCo}_y\text{Mn}_{2-y}\text{O}_4$  is investigated. The first order cooperative-normal-mode transition, detected through coefficient of thermal expansion, is found to disappear at a critical doping ( $y \sim 0.16$ ); interestingly, for  $y \gtrsim 0.16$  the resistivity does not change much with doping and the electrochemical capacity becomes constant over repeated cycling. The critical doping  $y \sim 0.16$  results in breakdown of the network of cooperative/coherent normal-mode distortions; this leads to vanishing of the first-order transition, establishment of hopping channels with lower resistance, and enhancing lithiation and delithiation of the battery, thereby minimizing electrochemical capacity fading.

The resistivity in  $\text{LiCo}_y\text{Mn}_{2-y}\text{O}_4$  can be expressed as follows

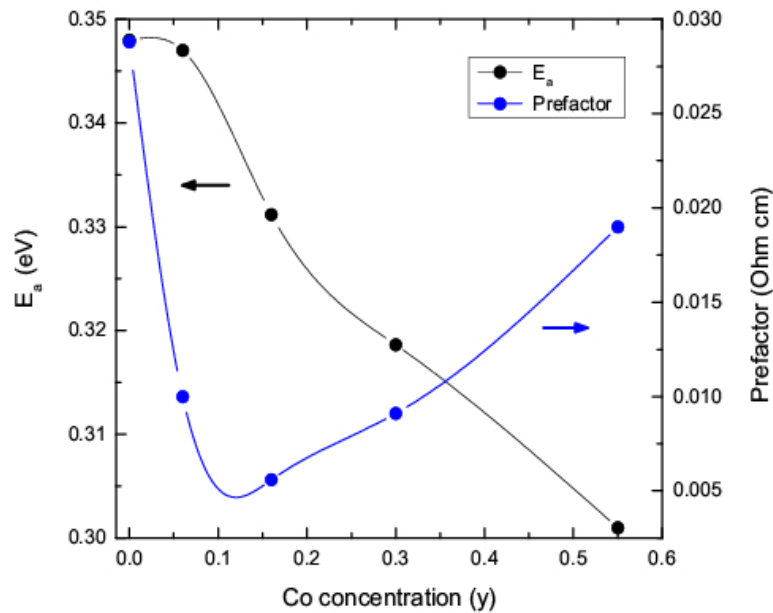
$$\rho = [A \exp(2R/\xi)/n] \exp(E_a/K_B T) \quad (3)$$

$A$  is a constant,  $n$  is the concentration of the  $e_g$  electrons,  $\xi$  is the localization length,  $R$  is the shortest hopping distance for an  $e_g$  electron (i.e., the distance between two neighboring  $\text{Mn}^{3+}$  and  $\text{Mn}^{4+}$  ions), and  $T$  is the temperature. Even upon doping with cobalt (where  $\text{Co}^{3+}$  replaces  $\text{Mn}^{3+}$ ), each  $\text{Mn}^{3+}$  has the same number of diagonally opposite  $\text{Mn}^{4+}$  ions for the  $e_g$  electron to hop to; this justifies using a fixed-hopping-distance model rather than a variable-hopping-range model.

**FIG. 9.** Linearity in plots of  $\log_{10}(\rho)$  vs  $1/T$  depicting activated transport at various dopings and above the structural transition. For doping below  $y \sim 0.16$ , the resistivity drops sizeably with increase in doping; contrastingly, for  $y \gtrsim 0.16$ , the resistivity does not change much with doping.



Our transport model is clearly verified by Fig. 9 which depicts linear plots of  $\log_{10}(\rho)$  versus  $1/T$ . Using Fig. 9, at various Co-doping values, we extract the prefactor  $A \exp(2R/\xi)/n$  and the activation energy  $E_a$  [occurring in Eq. (3)] and generate Fig. 10. Now, the cobalt doping has two competing effects on the localization length  $\xi$ : (i) the frustration (produced by electron-electron repulsion) decreases with increase in doping and, thus, tends to increase  $\xi$ ; (ii) contrastingly, the disorder effect due to doping tends to decrease  $\xi$ . However, at a critical doping  $y_c$ , there is a breakdown of the cooperative normal-mode-network and frustration is no longer significant to  $\xi$  for dopings beyond  $y_c$ . Thus, above  $y \sim y_c$ ,  $\xi$  decreases with increasing doping; on the other hand, below  $y \sim y_c$ ,  $\xi$  increases rapidly with doping. Furthermore,  $1/n$  increases gradually with doping. Hence, in the above expression for resistivity, the prefactor  $A \exp(2R/\xi)/n$  will have a minimum as a function of Co-doping. In fact, as depicted in Fig. 10, the minimum in the prefactor  $A \exp(2R/\xi)/n$  occurs at  $y \sim 0.16$  which leads us to estimate  $y_c \sim 0.16$ . Lastly, it is of interest to note that the resistivity drops sizeably with increasing doping until the doping-level attains a value  $y \sim 0.16$ ; at higher doping values (i.e.,  $y \gtrsim 0.16$ ), the resistivity does not change much (as can be seen in Fig. 9). This can be understood in terms of a non-cooperative network being established at  $y = y_c \sim 0.16$ ; above  $y_c$ , in Eq. (3) for resistivity, an increase in the prefactor  $A \exp(2R/\xi)/n$  is compensated by a reduction in  $\exp(E_a/K_B T)$ .



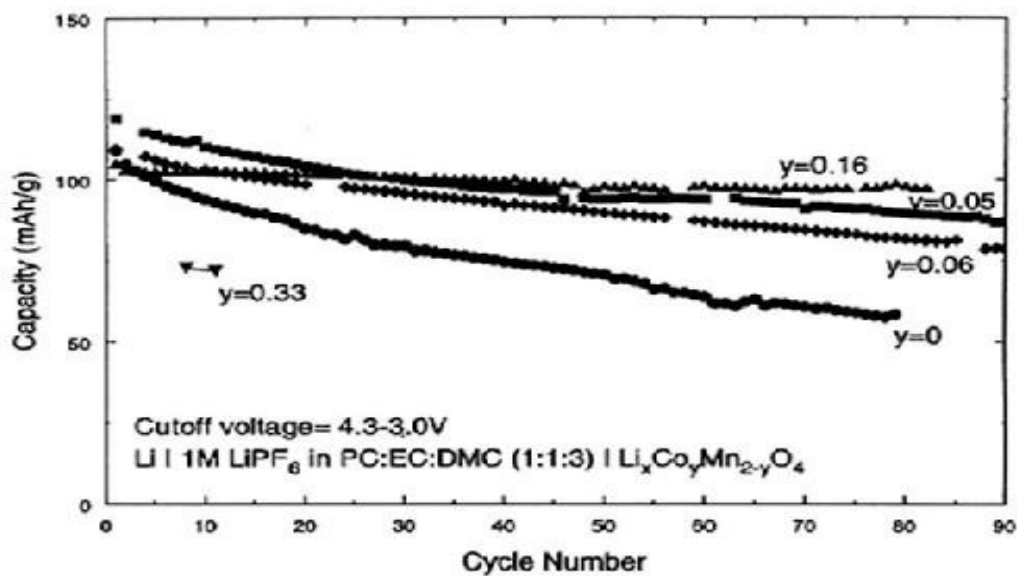
**FIG. 10.** Plots of the prefactor  $A \exp(2R/\xi)/n$  and the activation energy  $E_a$  [occurring in the resistivity equation (3)] as a function of cobalt doping in  $\text{LiCo}_y\text{Mn}_{2-y}\text{O}_4$ . The prefactor shows a minimum at  $y \sim 0.16$  and the drop in  $E_a$  is sharper till  $y \sim 0.16$ ; both are indicative of a change in the transport mechanism.

Finally, we will discuss capacity fading as displayed in Fig. 11. In the undoped case and at lower dopings (i.e.,  $y < 0.16$ ), the network of cooperative/coherent normal-mode distortions restricts



lithiation (delithiation) of the cathode material; consequently, each time only a fraction of the un-lithiated (lithiated) material gets lithiated (delithiated). On increasing the doping to  $y \gtrsim 0.16$ , a network of non-cooperative normal-mode distortions is established which facilitates both the lithiation and the delithiation processes. Thus, while there is capacity fading upon repeated cycling at lower values of doping (i.e.,  $y < 0.16$ ), the capacity remains constant for  $y \gtrsim 0.16$ . However, for  $y \gtrsim 0.16$ , at higher doping values the capacity is less due to decrease in the number of  $e_g$  carriers. Thus ideally, it is best to use  $\text{LiCo}_y\text{Mn}_{2-y}\text{O}_4$  at  $y \sim 0.16$  for optimal electrochemical performance.

**FIG. 11.** Variation of the capacity as a function of cycle number for  $\text{Li}/\text{LiCo}_y\text{Mn}_{2-y}\text{O}_4$  cells at various cobalt dopings. At higher doping  $y \sim 0.16$ , capacity remains unchanged after repeated cycling. Reproduced with permission from J. Electrochem. Soc. **145**, 807 (1998).



## **E) Study of two-spin entanglement in singlet states**

M. Q. Lone, A. Dey, and S. Yarlagadda, Solid State Communications 202, 73 (2015).

Valence-bond (VB) states were shown to be the ground states of spin systems earlier by C. K. Majumdar's group and later by Shastry and Sutherland. Any spin-singlet state (i.e., state with total spin eigenvalue  $\mathbf{S}_T = \mathbf{0}$ ) can be expressed as a superposition of VB states.

Correlation/entanglement between two spins plays an important role in understanding phase transitions, length scale in the system, etc. Although two-spin correlation/entanglement has been investigated in certain Resonating-valence-bond (RVB) states, to our knowledge, there has been no explicit construction of RVB states that would contain maximal entanglement of two-spin subsystems.

The spins of a two-spin singlet, while being maximally entangled with each other, are completely unentangled with the remaining spins and thus show monogamy. Thus, if we wish to establish greater entanglement between the two-spin subsystem and the rest of the spin system, we are forced to diminish entanglement between the spins of the two-spin subsystem. The purpose of this work is to enhance our understanding of the distribution of two-spin entanglement in singlet states. We analyze the following two extreme cases in a general singlet: (1) maximal average entanglement between two spins; and (2) maximal average entanglement between a two-spin subsystem and the remaining spins. The main results of this work are as follows. First, we study two-spin entanglement in singlets. We show that the average entanglement between two spins is maximum (as expected) for a single VB state. In a singlet, we also demonstrate that  $SU(2)$  isotropy and homogeneity (in spin-spin correlation function) maximize the bipartite entanglement  $E_v^2$  (the average entanglement between a subsystem of two spins and the rest of the system) while minimizing the average entanglement between two spins. Second, we adopt two ways of obtaining maximal  $E_v^2$  states: (1) imposing homogeneity on singlet states; and (2) generating isotropy in a general homogeneous state. By using these two approaches, we construct explicitly four-spin and six-spin highly entangled states that are both isotropic and homogeneous. Our maximal  $E_v^2$  states represent a new class of RVB states which we show to be the ground states of the infinite-range Heisenberg model.

## **Future Plans**

It would be great if the above proposals of a charge qubit and giant magnetoelectric effect in manganite-manganite heterostructures can be realized. In spite of India's strength in oxides, so far I have not been able to persuade experimentalists in India to realize them. After a fair amount of survey and search, I managed to convince Prof. R. Ramesh (Univ. of Berkeley, USA) to carry out the relevant experiments.

In future, I hope to gain further insights into the Lithium-based battery materials by interacting with the battery groups in India and at Argonne National Lab, USA.

I also would like to write books/reviews detailing the strong-weak duality transformation that we have devised and bring out its utility by considering various systems with strong electron-phonon interaction.

## **List of papers (2012-2017)**

**In all the works below, main contribution (main ideas, etc.) was by me.**

**1) Correlation between battery material performance and cooperative electron-phonon interaction in  $\text{LiCo}_y\text{Mn}_{2-y}\text{O}_4$ ,**

Krishna Rao Ragavendran, P. Mandal, and S. Yarlagadda, Appl. Phys. Lett. **110**, 143901 (2017).

**2) Checkerboard-supersolidity in a two-dimensional Bose-Holstein model,**

Satyaki Kar and S. Yarlagadda, Annals of Physics **375**, 322 (2016).

**3) Decoherence dynamics of interacting qubits coupled to a bath of local optical phonons,**

Muzaffar Q. Lone and S. Yarlagadda, Int. J. Mod. Phys. B **30**, 1650063 (2016).

**4) Study of decoherence in models for hard-core bosons coupled to optical phonons,**

Amit Dey, Muzaffar Q. Lone, and S. Yarlagadda, Phys. Rev. B **92**, 094302 (2015).

**5) Study of two-spin entanglement in singlet states,**

Muzaffar Q. Lone, Amit Dey, and S. Yarlagadda, Solid State Communications **202**, 73 (2015).

**6) An analysis of the  $t_2 - V$  model,**

Amrita Ghosh and S. Yarlagadda, Phys. Rev. B **90**, 045140 (2014).

**7) Polaron dynamics and decoherence in an interacting two-spin system coupled to optical phonon environment,**

Amit Dey and S. Yarlagadda, Phys. Rev. B **89**, 064311 (2014).

**8) A study of cooperative breathing-mode in molecular chain,**

Ravindra Pankaj and Sudhakar Yarlagadda, Phys. Rev. B **86**, 035453 (2012).

**9) Correlated singlet phase in the one-dimensional Hubbard-Holstein model,**

Sahinur Reja, Sudhakar Yarlagadda, Peter B. Littlewood, Phys. Rev. B **86**, 045110 (2012).

**10) Giant magnetoelectric effect in pure manganite-manganite heterostructures,**

Sanjukta Paul, Ravindra Pankaj, Sudhakar Yarlagadda, Pinaki Majumdar, and Peter B. Littlewood, arXiv:1702.06302 (under review).

**11) Temperature dependence of long coherence times of oxide charge qubits,**

Amit Dey and S. Yarlagadda, arXiv:1610.01866 (under review).

**12) Study of long-range orders of hard-core bosons coupled to cooperative normal modes in two-dimensional lattices,**

A. Ghosh and S. Yarlagadda, arXiv:1610.01447 (under review).

**13) Charge and orbital order due to cooperative Jahn-Teller effect in manganite chains,**

Ravindra Pankaj and S. Yarlagadda, arXiv:1608.06055 (submitted).

## **Invited Talks at International/Nat. conferences/workshops, 2012-2017:**

- 1) **Plenary lecture on "Oxide devices – the best replacement for semiconductor devices?"** at the International meeting on "Highly Correlated Systems-IMHCS-2017" at Mahatma Gandhi Univ., Kerala, 24-26 March 2017.
- 2) **"Oxide double quantum dot: an answer to the qubit problem?"** at the "International meeting on quantum information processing and applications" Harish-Chandra Research Institute, Allahabad (India); Dec. 7-13 (2015). **(Invited Talk).**
- 3) **Key-note invited talk on "Oxide devices -- the next revolution"** at the National Seminar (2014) on "Recent Advances in Physics" at Berhampur Univ. jointly organized by Berhampur Univ. and IOP (Bhubaneswar).
- 4) **"Polaron dynamics and decoherence in an interacting two-spin system coupled to optical phonon environment"** at the "International meeting on quantum information processing and applications" Harish-Chandra Research Institute, Allahabad (India), Dec. 2-8, 2013. **(Invited Talk).**
- 5) **"Modeling multiferroicity in manganite heterostructures by including cooperative electron-phonon interaction"** at the Indo-Japan discussion meeting, entitled "New functionalities in electronic and magnetic materials", SSCU, IISc, October 18-20, 2012. **(Invited Talk).**
- 6) **"Strong multiferroicity and giant magnetoelectric effect in (Insulator)/(LaMnO<sub>3</sub>)<sub>n</sub>/(SrMnO<sub>3</sub>)<sub>n</sub>/(Insulator) heterostructure"** at the international conference on "Correlated Oxides: novel quantum states, device physics and energy technologies" March-April 2012, Cambridge Univ. **(Invited Talk).**

## **Colloquiums/Seminars at National/Foreign Univs./Institutes (2012-2017):**

- 1) **"An analysis of the extremely anisotropic next-nearest-neighbour Heisenberg Model"** at IMSC (Chennai) on 4/Feb./2014.
- 2) **"Polaron dynamics and decoherence in an interacting two-spin system coupled to optical phonon environment"** at I.I.T. Madras on 30/Jan./2014.
- 3) **Colloquium on "Oxide electronics -- an answer to the miniaturization challenge?"** at IISER Bhopal on 4/Sept./2015.
- 4) **"Oxide double quantum dot -- an answer to the qubit problem?"** Condensed Matter Seminar, Physics dept., Purdue Univ.; 19/Feb./2016.
- 5) **"Oxide systems -- an answer to the qubit problem?"** Material Science Seminar, Argonne National Lab; 2/March/2016.
- 6) **"Oxide systems -- an answer to the qubit problem?"** Condensed Matter Seminar, Physics dept., Univ. of Illinois at Urbana-Champaign 10/March/16.

### **Special distinctions/visits:**

Visiting Scholar at Argonne National Lab, USA for 2 Months from Jan./16 to March/16

### **Other academic records besides research and development (e.g. teaching)**

- 1) Taught an advanced condensed matter physics course (using path-integral approach) at SINP (in 2012-2013) from Altland and Simon's book on Condensed Matter Field Theory. The students were asked to solve research-type problems in areas of magnetism, superconductivity, superfluidity, electron gas, etc.
- 2) I taught a Post MSc course on advanced quantum mechanics in the first semester (Aug.-Nov., 2014).
- 3) I offered a Post MSc reading course on advanced condensed matter physics in the third semester (2015).

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### **PhD Thesis Examiner for the following students:**

- 1) Ashis K. Nandy (Nov./2013, S. N. Bose, Supervisor: Prof. P. Mahadevan)
- 2) Sudipta Kanungo (Nov./2013, S. N. Bose, Supervisor: Prof. Tanusri Saha-Dasgupta)
- 3) Kapil Gupta (Aug./2013, S. N. Bose, Supervisor: Prof. P. Mahadevan)

### **Other academic activity:**

- 1) I have supervised several PhD student reviews at SINP.
- 2) I have also served as an examiner for several PhD student reviews at SINP.
- 3) Several times I have set entrance exam questions and also served on PhD interview boards at SINP.
- 4) I have organized several colloquiums, lectures, and seminars at SINP.

### **Faculty evaluation committee member:**

- 1) I was on the review committee in Nov./2016 for considering the extension of an ex-faculty member of S. N. Bose Center for the position of a Visiting Associate Professor.
- 2) I was expert member of selection committee for selection of Associate/Assistant Professors in the Department of Physics at IIT Bombay on 22/April/2016.
- 3) I was an expert evaluator for the research performance of an assistant professor in dept. of physics of Indian Institute of Space Science and Technology (IIST) in Nov./2016.

### **Postdoc evaluation committee member:**

I was the external expert (a member of the Selection Committee) for the Post Doctoral Research Associateship Program at the S N Bose Center; meeting held on 2/Aug./2016

### **PhD committee member:**

I am the external expert of the thesis committee of Mr. Hrishit Banerjee, SRF, working under the supervision of Prof. Tanusri Saha Dasgupt and Dr. Manoranjan Kumar at S. N. Bose Center

I am on the PhD committee for 1 of Prof. K. Pradhan's students (S. Chakraborty), 2 of Prof. Milan Sanyal's students ( A. B. Dey, and A. Singh), and 2 of Prof. Chandan Mazumdar's students (S. Mandal and M. Kundu); was on the PhD committee for 2 of Prof. Arti Garg's students (S. Nag and G. Majumdar).

### **Research planning, management, and organising experience:**

- 1) I am the head of the Condensed Matter Physics division.
- 2) I am a member of the SINP Scientific Council and help in making important decisions in the institute (regarding various norms pertaining to faculty, students, and other employees).
- 3) I am the project co-ordinator for the XII five-year (2012-2017) plan and beyond for condensed matter physics project; I helped in the formulation and the defense of the project.
- 4) I am the convener for the faculty search committee (FSC). I help in making important decisions regarding faculty hiring at SINP.
- 5) I also take active interest in the searching and the hiring of good new faculty members for the CMP division.
- 6) I am also the coordinator of the Joint International PhD program at SINP.
- 7) I am also a member of the center for advanced research & education (CARE) committee.
- 8) I also started (with the help of Prof. P. B. Littlewood, Prof. B. K. Chakrabarti, and Prof. M. K. Sanyal) a joint PhD program between SINP and Cavendish Lab (with PhD degree to be given by Univ. of Cambridge). I helped in the formulation and signing of Saha-Cavendish fellowship program. I helped SINP students in the selection process of the Saha-Cavendish fellowship.

### Reception and recognition of research contributions accorded by other researcher workers.

We derived a quasiparticle pseudo Hamiltonian of an infinitesimally polarized electron gas which fully takes into account the many-body effects of both charge and spin density fluctuations. We calculated self-consistently Fermi liquid parameters like the effective mass, the effective g-factor, spin susceptibility in two-dimensional systems and found reasonable agreement with experiments. My works on electron gas [see especially PRB **38** 10966 (1988); PRB **40** 5432 (1990); PRB **49** 7887 (1994); PRB **49** 14188 (1994)] are well recognized and distinguished scientists (including Nobel prize winners) cite these works. In fact G. F. Giuliani and G. Vignale have written a book ["Quantum Theory of the Electron Liquid" (Cambridge, 2005)] in which my work forms a major theme of Chapter 8.

I had included effects of electron-impurity interactions [PRB **44** 13101 (1991)] and showed that the magnetization instability (at filling factor 2 in the quantum Hall regime) predicted by Giuliani and Quinnin [PRB **31** 6228 (1985)] does occur; the experiment (measuring diagonal resistivity in GaInAs-InP heterostructures) I proposed was carried out by K. von Klitzing *et al.* [Phys. Rev. B **47** 4048 (1993)] and the instability was explicitly demonstrated. The prediction was also verified by Mike Pepper *et al.* [PRL **79**, 4449, (1997)] through activation transport studies. Several Nobel prize winners (such as H. L. Stormer, D. C. Tsui, K. v. Klitzing, and H. Kroemer) and Buckley award winners (such as Jainendra Jain, Allan MacDonald, etc.) cite this work.

### Any other relevant information:

Guest Editor (along Prof. Peter B. Littlewood) for EPJ B topical issue: "Coexistence of long-range orders in low-dimensional systems" to be published later this year.

### Organized the following memorial lectures (2012-2017):

- 1) JC Bose Memorial lecture during March/April 2013 by Prof. G. Baskaran.
- 2) Cockcroft-Walton Lecture in April/2013 by Prof. Michael Pepper.
- 3) Organized a JC Bose Memorial lecture by Prof. R. Rosner (Univ. of Chicago) on 4/Feb./2015 at SINP.
- 4) Organized a Saha Memorial Lecture by Prof. T. V. Ramakrishnan (IISc) on 8/July/2015 at SINP.
- 5) Helped organize a J C Bose Lecture by Prof. Jogesh Pati (Stanford University, USA) on 14/January/2016 at SINP.

### **Referee work:**

I was a referee for Phys. Rev. Lett., Phys. Rev. B., Pramana, EPJAP, EPJP, EPJ B, and Solid State Communications.

### **Chaired sessions in the following:**

- 1) International meeting on "Quantum information processing and applications" Harish-Chandra Research Institute, Allahabad (India), Dec. 2-8, 2013.
- 2) International conference on "Correlated Oxides: novel quantum states, device physics and energy technologies" March-April 2012, Cambridge Univ.
- 3) International meeting on "Quantum information processing and applications" Harish-Chandra Research Institute, Allahabad (India); Dec. 7-13 (2015).
- 4) International meeting on "Highly Correlated Systems-IMHCS-2017" at Mahatma Gandhi Univ., Kerala, 24-26 March 2017.



# **National Level Academic Review**

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**Surface Physics and Material Science (SPMS) Division**

***A Report for the period 2012-2017***

## Present Staff

<b>Faculties/Scientists (12)</b>	<b>Sc. Officers/Assistants/Technicians (7)</b>
Alokmay Datta, Senior Prof . H+	Avijit Das, Sc. Officer D
Satyanjan Bhattacharyya, Senior Prof. H, Head	Subir Roy, Sc. Officer D
Tapas Kumar Chini, Prof. G	Souvik Banerjee, Sc. Assistant D
Sangam Banerjee, Prof. G	Gautam Sarkar, Sc. Assistant D
Manabendra Mukherjee, Prof. G	Debraj Dey, Sc. Assistant C
Satyajit Hazra, Prof. G	Ramkrishna Dev Das, Sc. Assistant B
Krishnakumar S.R. Menon, Prof. G	Syamaprasad Mallik, Technician G
Satyaban Bhunia, Asso. Prof. F	
Madhusudan Roy, Asso. Prof. F	<b>Administrative/Auxiliary (3)</b>
Supratic Chakraborty, Asso. Prof. F	Mukul Ch. Das, AAO
Biswarup Satpati, Scientist F	Gobardhan Jana, Helper C
Mrinmay K. Mukhopadhyay, Asso. Prof. E	Prabhas Halder, Helper E

## Superannuated Staff

<b>Faculties (4)</b>	<b>Technician (1)</b>
Milan K. Sanyal, 2016	Sushanta Banerjee, 2017
Purushottam Chakraborty, 2015	
Srinanda Kundu, 2014	<b>Auxiliary (1)</b>
Debabrata Ghose, 2014	Harendranath Jana, 2015

## Present Postdoctoral Fellows (PDFs)

	Name of PDFs	Year of joining
1	Somnath Mahato	2016
2	Dhrubojyoti Roy	2016

## Present Research Fellows (RFs)

	Name of RFs	Year of joining	Ph.D. Supervisor(s)
1	Tapas Ghosh	2012	Biswarup Satpati
2	Arpan Maiti	2012	Tapas Kumar Chini
3	Achyut Maity	2012	Tapas Kumar Chini
4	Gouranga Manna	2012	Milan K. Sanyal
5	Barnamala Saha	2012	Sangam Banerjee
6	Arnab Singh	2013	Milan K. Sanyal & Mrinmay K. Mukhopadhyay
7	Gourab Bhattacharjee	2014	Biswarup Satpati
8	Anway Pradhan	2014	Satyaban Bhunia
9	Suman Mukherjee	2014	Satyaban Bhunia
10	Abhijit Roy	2016	Biswarup Satpati
11	Mantu Modak	2016	Sangam Banerjee
12	Bibhutibhusan Jena	2016	Krishnakumar S. R. Menon
13	Abhishek Rakshit	2016	Supratic Chakraborty
14	Pintu Barman	2017	Satyaranjan Bhattacharyya

## Ph.D. Degree Awarded (2012-todate)

	Name of RFs	Award	Ph.D. Supervisor	Present Occupation
1	Rupak Banerjee	2012	Milan K. Sanyal & Satyajit Hazra	Asst. Professor, IIT Gandhinagar
2	Smita Mukherjee	2012	Alokmay Datta	CSIR-Pool Scientist, CGCRI, Kolkata
3	Biswajit Saha	2012	Purushottam Chakraborty	Faculty, IEM, Saltlake, Kolkata
4	Suman Mandal	2012	Krishnakumar S. R. Menon	INSPIRE Faculty, IISc-Bengaluru
5	Mojammel Haque Mondal	2012	Manabendra Mukherjee	Faculty, IEST, Shibpur
6	A.K.M. Maidul Islam	2012	Manabendra Mukherjee	Faculty, Aliah Univesity, Kolkata
7	Sanjoy Kumar Mahata	2013	Krishnakumar S. R. Menon	Postdoc, University of Aarhus, Denmark
8	Sumistha Das (ISI-Kolkata)	2013	Arunava Goswami (ISI) & Alokmay Datta	Assistant Professor, Amity University, Haryana
9	Debasis Roy (Visva-Bharati)	2013	A. Bhattacharjee (VB) & Madhusudan Roy	
10	Sirshendu Gayen	2014	Milan K. Sanyal	Postdoc, IISER-Mohali
11	Nupur Biswas	2014	Alokmay Datta	Postdoc, RRI, Bengaluru
12	Manjula Sharma	2014	Milan K. Sanyal	Postdoc, IIT-Delhi
13	Pabitra Das	2014	Tapas Kumar Chini	Postdoc, Univ. Paris-Sud, France
14	Tanusree Samanta	2014	Manabendra Mukherjee	Scientist, Govt. of India, Pune
15	Satyaranjan Haldar	2014	Satyaban Bhunia	
16	Anuradha Bhattacharya	2015	Sangam Banerjee	Postdoc, RRI, Bengaluru
17	Abhishak Sharma	2015	Milan K. Sanyal	Postdoc, DESY-Germany
18	Paramita Chatterjee	2015	Satyajit Hazra	
19	Haradhan Mandal (Visva-Bharati)	2015	A. Bhattacharjee (VB) & Madhusudan Roy	
20	Jayanta Das	2015	Krishnakumar S. R. Menon	Faculty, Techno India Univ., Kolkata
21	Sumona Sinha	2016	Manabendra Mukherjee	Postdoc, S N Bose Centre, Kolkata
22	Amlan Roj (Visva-Bharati)	2016	A. Bhattacharjee (VB) & Madhusudan Roy	
23	Tanmay Ghosh	2016	Biswarup Satpati	Postdoc, National University

				of Singapore
24	Safiul Alam Mollick	2016	Debabrata Ghose	Postdoc, IIT-Roorkee
25	Koushik Bagani	2016	Sangam Banerjee	Postdoc, Weizmann Institute, Israel
26	Mayukh Kumar Roy	2016	Sangam Banerjee	Postdoc, University of UAE, Dubai
27	Ishani Roy	2016	Satyajit Hazra	
28	Shantanu Maiti	2016	Milan K. Sanyal	Postdoc, Universität Tübingen, Germany
29	Debasree Chowdhury	2017	Debabrata Ghose	
30	Suvankar Chakraborty	2017	Krishnakumar S. R. Menon	Faculty, Haldia Inst. Technology, Haldia (W.B.)
31	Kaustabh Dan	2017	Alokmay Datta	
32	Uttam Kumar Basak	2017	Alokmay Datta	Postdoc, IISc, Bengaluru
33	Sk Abdul Kader Md Faruque	2017	Supratic Chakraborty	

### Ph.D. Thesis Submitted

	Name of RFs	Year	Ph.D. Supervisor	Status
1	Debaleen Biswas	2016	Supratic Chakraborty	
2	Ashish K. Kundu	2017	Krishnakumar S. R. Menon	Postdoc, ICTP, Italy
3	Madhumita Choudhuri	2017	Alokmay Datta	
4	Shyamal Mondal	2017	Satyaranjan Bhattacharyya	Faculty, Maharaja Manindra Chandra College, Kolkata

### Ph.D. Thesis to be submitted

	Name of RFs	Ph.D. Supervisor	Status
1	Mala Mukhopadhyay	Satyajit Hazra	Asst. Professor, Haldia Inst. Technology, Haldia (W.B.)
2	Arpan Bhattacharyya	Milan K. Sanyal	
3	Arka Bikash Dey	Milan K. Sanyal	
4	Rajendra Prasad Giri	Mrinmay K. Mukhopadhyay	
5	Sukanta Barman	Krishnakumar S. R. Menon	Asst. Professor, Raja Peary Mohan College, Hooghly (W.B.)

## Important equipment and facility

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### Growth Facilities:

- RF/DC Magnetron Sputtering unit
- Langmuir-Blodgett Trough, Spin Coater
- High current ion implanter
- Low energy high current ion beam, low energy negative ion implanter
- Molecular Beam Epitaxy (MBE)
- Metal Organic Vapor Phase Epitaxy (MOVPE)
- Size-selected Nanocluster Deposition
- Clean Room facilities of Class 100 and 1000 grades
- UV-Photolithography system

### Characterization Techniques:

- Grazing Incidence X-ray Scattering (GIXS) techniques such as XR, GISAXS, GID, EXAFS, etc. using Laboratory as well as Synchrotron sources
- Dynamic Light Scattering (DLS)
- Scanning Electron Microscopy (SEM) augmented with EDX & EBSD
- 300 kV Transmission Electron Microscopy (TEM) with EDX & EELS
- Scanning Probe Microscopy (Ambient SPM, VT UHV-SPM, Nano-indentation)
- Brewster Angle Microscopy (BAM)
- Spectroscopy (XPS/UPS/AES, ARPES, UV-Visible, Raman, PL/CL)
- Ion Microbeam Techniques (SIMS/SNMS)
- Magnetic measurements (SQUID, MOKE)
- Physical property measurement systems (PPMS)

## Research highlights (last 5 years and future plan)

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Surface Physics and Materials Science (SPMS) Division is pursuing cutting-edge research in the frontline areas of growth, characterization, physical/chemical properties, functionalization and applications of surfaces/interfaces, thin films and nanomaterials during the last 5 years. In order to achieve superior device performances, it is absolutely necessary to explore the properties of new materials within multifunctional platforms in the nanometer length scale (~1-100 nm), where the surface and the interface essentially dictates the functions. Thus, finding different routes for growing nanomaterials of unique morphologies and properties along with their detailed characterizations such as structure, composition, electronic and magnetic structures with high degree of spatial/spectral resolution is essential for their basic understanding and for technological applications. This has been the driving force behind the research activities of the SPMS Division for the last 5 years to address important issues related to the growth of low-dimensional metallic/semiconducting/organic thin films, nanoparticles and nanocomposite materials using advanced physical and chemical routes. Further extensive characterizations are carried out with state-of-the-art techniques for achieving tunable mechanical/electrical/magnetic/optical properties relevant for applications in diverse areas of micro-nano science and technology. During the last 10-15 years, SPMS division has set up many advanced experimental facilities and has generated a strong research base in this area through significant funding from Department of Atomic Energy (DAE), keeping in focus the futuristic developments and the fast pace of progress in the fields of

nanoscience and surface physics. So, the faculty members of SPMS division, with their diversified fields of expertise, have been working on systems where surface/interface plays a crucial role in dictating its properties relevant to applications, such as, MOS-based electronic devices, magnetic devices, photonic devices, sensors for detecting hazardous gas and human blood glucose monitoring, bio-imaging, solar cells, to name a few. Many faculty members of the division have also been using advanced synchrotron facilities in India and abroad for a further detailed understanding of these materials, apart from developing an SINP beamline at the INDUS II synchrotron at RRCAT, Indore.

## Future Plan

We have identified 3 different areas where the faculties of the SPMS division will be actively pursuing in the medium and long term vision. These are i) Working towards the development of energy harvesting materials, mainly towards solar photovoltaics ii) Setting up a Centre of Excellence for Surface and Interface Science (CESIS) at SINP with state-of-art facilities for nanoscience research. iii) Advanced new material research using synchrotron radiation sources, especially using the SINP beamline at INDUS-II.

The four major thrust areas for the energy harvesting materials have been identified as (i) Growth of organic solar cells (OSCs), (ii) Growth of III-V compound semiconductor based high efficiency multijunction solar cells, (iii) Oxide compound based energy harvesting materials and (iv) Advanced solar cell materials based on plasmonic metal nanoparticles with patterned and complex structures including size-selected nanoclusters, nano-composites and dendritic structures. For the energy harvesting materials, ultrathin film materials will be studied where photovoltaic, piezoelectric, thermoelectric and pyroelectric properties are important. Detailed structural and property characterizations of these grown materials will be performed using our existing as well as the proposed facilities. New methods for enhancing the efficiency of thin-film solar cells, such as light trapping using plasmon-enhanced local electromagnetic field from metallic nanostructures, metallic/dielectric nanoparticles and employing organo-metallic structures will be explored.

Cutting-edge science and technology in the 21st century relies heavily on the availability of advanced characterization techniques, which are lacking in the country for the basic, applied as well as for the industrial research. SPMS division is already a leading group in India for the study of *surface and interface physics*. Faculties of this division are experts in a wide variety of surface and interface characterization techniques, which are especially useful for the study of low dimensional systems or nanomaterials having large surface to volume ratio. Setting up of the CESIS at SINP with a variety of state-of-the-art microscopy, spectroscopy and X-ray scattering facilities will enable us to perform front-ranking experiments with the aim of developing advanced functional devices. As a first step, utilizing our long standing experience in grazing incidence X-ray scattering (GAXS), in general and *synchrotron experience in GISAXS techniques* (of about 20 years), in particular, we want to *develop* a dedicated SAXS/GISAXS/WAXS *laboratory facility*, to determine the morphology and growth of nanostructured and mesostructured materials. To understand the nanoscale transport, magnetic, and electronic properties, site-specific measurements must be carried out using the highest possible spatial resolution using insitu high resolution transmission electron microscopy.

We also want to carry out research on new advanced materials in the field of nanoscience and nanotechnology using synchrotron facilities available throughout the world and also using SINP beamline at INDUS II, RRCAT, which is under development. The latter once developed as grazing incidence scattering facility, will be upgraded to accommodate other experimental facilities. In order to make this beamline very versatile, it is planned to extend the diffraction measurements in a wide temperature range from 4K to 1200K using a closed-cycle cryostat and a high-temperature cell. It is also planned to set up UHV based thin film growth system to perform on-line *in-situ* growth studies. To significantly improve the fast detection of the scattered beam, a pixel based high sensitive 2D detector and a highly efficient point detector with low background noise will be used.

## Important Results

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- **Morphology and structure at surfaces and interfaces - Transmission Electron Microscopy studies**

It is known that functional properties of the novel materials in nanometer length scales depend on atomic scale order and electronic structure. Therefore, probing the microstructural aspects, like lattice defects, grain boundaries, and compositional variation at near atomic level spatial resolution as well as the electronic structure, are essential to understand the basic science of condensed matter in low-dimensional regimes. These, in turn, provide the inputs towards the significant advancement for developing future electronic devices and new materials. The thrust in our research during last 5 years has been to explore these aspects and to address a few important issues that are related to growth, structural and optical properties of noble metal nanostructures synthesized *via* chemical routes. These nanomaterials have been characterized extensively by a modern state-of-the-art 300 kV transmission electron microscope (TEM) equipped with associated analytical techniques with the capability of giving sub nanometer spatial and few eV energy resolution chemical/electronic structural information in addition to providing routine atomic resolution crystalline structural information in real and reciprocal space. The central motivation of our works is to understand the role of structural parameters, such as crystal orientation, crystal defects/strain on the growth mechanism of the nanoparticles. With the help of crystallographic relationship between the seed (nucleation centre) and the finally grown nanostructure, we have been able to elucidate the growth mechanism of nanoparticles with various morphologies. We have established the fact that the defect induced growth process [*J. Phys. Chem. C* 2013, **117**, 10825] can be taken as a general growth mechanism to explain the formation of triangular Au, Ag or combined Au-Ag core-shell nanoprisms, nanorods, etc. Our in-depth structural characterization has revealed the crucial role of ascorbic acid towards the fabrication of continuous bimetallic nanorings grown at room temperature [*J. Mater. Chem. C* 2014, **2**, 2439]. Moreover, we have demonstrated a new type of heteroepitaxy [*Phys. Chem. Chem. Phys.* 2014, **16**, 16730] during the investigation of growth process of Ag nano-inukshuk structures on germanium surface, where the large lattice mismatch between epilayer (silver) and substrate (germanium) is accommodated at the interface by the formation of low-energy asymmetric tilt boundaries. The phenomenon of tilted heteroepitaxial growth as observed in the present analysis is remarkable. It violates our general wisdom on the basic mechanism of the solid state growth process. That an atomically sharp interface (revealed by cross-sectional TEM) plays a crucial role in determining the quality of the cutting-edge new materials having possible applications in next generation electronic, spintronic and quantum computation devices, has recently been demonstrated in a high-temperature ferromagnetic topological insulator utilizing our TEM facility through an international collaborative work [*Nature* 2016, **533**, 513]. Our TEM work has been instrumental in the discovery of a super dense nonmagnetic fcc phase of cobalt [*Scientific Reports* 2017, **7**, 41856] and demonstrating the growth of nanoscale nickel monosilicide [*J. Appl. Phys.* 2017, **121**, 045302], a desired material for the future complementary metal oxide semiconductor (CMOS) technology.

- **Surface nature/energy driven growth of the low dimensional structures**

The substrate surface natures (namely, the free energy, the polar/nonpolar or electrostatic nature), initially and after evolution with time, are known to play strong role in the growth and stability/instability of the low dimensional structures (ideal for testing basic physics and have promising applications in different fields) onto it. However, in order to understand the exact role, nondestructive surface/interface sensitive techniques are essential. Here complementary grazing incidence X-ray scattering (GIXS) and scanning probe microscopy (SPM) techniques have been utilized successfully to understand the growth and stability of the low dimensional structures and the role of surface/interface on it. For example, it has been observed that the cylindrical shaped micelles,



which are initially circular on a hydrophilic OH-terminated Si substrate in order to form a perfect 2D-hexagonal structure, become elliptical (extended along the in-plane) on a hydrophobic H-terminated Si substrate to form a slightly compressed 2D-hexagonal structure due to a different attachment of the film to the substrate [*Soft Matter* 2012, **8**, 2856]. The Cl-terminated Si surface, which was slightly controversial, was studied and found weak hydrophilic in nature [*Soft Matter* 2013, **9**, 9799]. However, it transforms toward weak-hydrophobic with time due to the growth of less homogeneous oxide layer [*J. Phys. Chem. C* 2014, **118**, 11350]. The crystalline ordering of poly(3-dodecylthiophene) [P3DDT] films, which is of immense importance in their performance as semiconducting materials (as it influence the charge delocalization), is found to depend strongly on the type (viscosity and evaporation rate) of good solvent, both near the film-substrate interface and above it [*Soft Matter* 2015, **11**, 3724] and also on the addition of poor solvent through coil-like to rod-like transition of P3DDT molecules and subsequent  $\pi$ - $\pi$  stacking due to thermal annealing [*RSC Adv.* 2015, **5**, 665]. Formation of 2D-networked structures of disk-like islands for ultrathin Langmuir-Schaefer (LS) films of thiol-coated Au-nanoparticles (DT-AuNPs) on H-passivated Si substrates is evidenced for the first time, directly from a broad peak in grazing incidence small angle X-ray scattering (GISAXS) data and also from atomic force microscopy (AFM) images [*RSC Adv.* 2016, **6**, 12326]. The structural information of the LS films, obtained at different surface pressure, helps to infer the growth of Langmuir monolayers of DT-AuNPs, which is very important in understanding the self-assembly process of nanoparticles at the air-water interface and in controlling the growth of 2D-networked nanostructures in large areas.

- **Electronic structure and magnetism of surfaces and thin films**

Study of electronic structure and magnetism of surfaces and thin films are very important in their basic understanding as well as for their applications in various futuristic functional devices. Our studies have been focused on the epitaxially grown ultrathin films of metals, strongly correlated metal-oxides and overlayers, surfaces of single crystals of oxides as well as layered chalcogenide materials. It is important to study the surface structure of these materials, as it determines their electronic structure as well as magnetic properties. For the study of these surface properties, we employ various surface-sensitive tools, including electron and x-ray spectroscopic techniques, scattering techniques as well as spectromicroscopic techniques. For the study of surface structure, we primarily use Low Energy Electron Diffraction (LEED), while for the electronic structure studies we use X-ray Photoemission Spectroscopy (XPS) as well as Angle-Resolved Photoemission Spectroscopy (ARPES) techniques. For surface magnetism studies, we use various synchrotron-based spectroscopic methods such as X-ray Magnetic Circular Dichroism (XMCD) for ferromagnetic materials while for antiferromagnetic materials we use the X-ray Magnetic Linear Dichroism (XMLD) technique. We have also developed a method to study the surface antiferromagnetism using the exchange-scattered electrons within the Low Energy Electron Diffraction (LEED) set up. We have been very successful in elucidating the surface electronic structures, magnetic structures and their structural and morphological origins in correlation to each other for a large number of strongly correlated model systems. In order to reach a microscopic understanding of these systems, we have undertaken extensive spectromicroscopic studies using Low Energy Electron Microscopy (LEEM) and Photoemission Electron Microscopy (PEEM) techniques. We have performed extensive studies of the antiferromagnetic NiO single crystals and ultrathin films using XPS, ARPES, LEED, LEEM, XMLD-PEEM methods and have been the subject of many publications. Electronic band structures of low-dimensional layered materials such as single crystal Graphite, MoS<sub>2</sub>, MoSe<sub>2</sub> etc. have also been extensively investigated. Epitaxial Cr, V and Mn monolayers, and multilayers, as well as their oxides such as V<sub>2</sub>O<sub>3</sub>, MnO, Mn<sub>3</sub>O<sub>4</sub> etc, have been studied in respect of their surface magnetism and electronic structures. Further systems studied includes ultrathin films and overlayers of CoO, MgO, Cu<sub>2</sub>O, metallic Sn and SnO etc.

- **Size-selected metal nanocluster deposition to get functional thin films**

A customised nanocluster deposition facility with *in situ* XPS attachment in the main chamber has been installed successfully for the fabrication of thin films of size-selected metal nanoclusters. Different parameters of the cluster source have been optimised to get the optimal condition for its operation. Novel properties of clusters depend on their sizes. For example, it has been found that the size of a cluster is crucial factor for their catalytic activity. Similar argument applies to the applications in magnetic, electric or transport properties. It is, therefore, important to get size-dependent clusters and films composed of monodispersed clusters on substrates for applications or studies of various novel properties of nanoclusters. We deposited size-selected (diameter ~3 nm) Cu and Ag nanoclusters on a variety of substrates with very low kinetic energy to keep the clusters intact with respect to their shapes and sizes as compared to clusters in flight condition in the magnetron based gas aggregation type source equipped with a quadrupole mass filter (QMF) that selects sizes of clusters before landing. TEM study shows that the size-distributions of isolated islands peaks around the selected size of clusters and consequently the diffusion of these nano-scale islands is very low. In another study, the oxidation dynamics of a copper nanocluster film, containing fractal islands of size-selected soft-landed nanoclusters with an average diameter of 3 nm has been carried out. The time evolution of the spontaneous oxidation of the prepared film in air at room temperature (RT) was studied. A compositional analysis of the film was carried out in an ultra-high vacuum (UHV) deposition chamber using an *in situ* XPS system. The morphological aspects of the deposited film were studied with a high resolution scanning electron microscope (SEM) and an atomic force microscope (AFM). We report the spontaneous production of highly pure (95%) and technologically appealing nano-crystalline Cu<sub>2</sub>O within 300 seconds of air exposure. The crystalline structure was probed using high resolution TEM (HRTEM) and the optical properties were studied using a cathodoluminescence (CL) device attached to a SEM. Apart from these studies, growth dynamics of films composed of size-selected metal nanoclusters on various substrates are being studied.

- **Metalorganic Vapour Phase Epitaxial (MOVPE) growth of compound semiconductor and nanomaterials**

The main focus of our research is to initiate work on growth of multi-junction tandem solar cell structure. These solar cells have the potential to achieve very high efficiency, more than 50 % as compared to ~15% for Si. This is the high time to target this research in India to match the current scenario and demand in the country. Metalorganic Vapour Phase Epitaxy (MOVPE) growth methodology is typically used to develop the core photovoltaic materials used in the cells. After installation of the MOVPE system, we have successfully grown epitaxial structures such as AlAs/GaAs multilayer Bragg reflector which was designed to get selective optical reflection at the green region of the spectrum. Such Bragg reflectors are important in fabricating multi-junction solar cell structures. We have also grown Al<sub>0.3</sub>Ga<sub>0.7</sub>As/GaAs multi quantum wells (MQWs) structures with nominal thicknesses 35 Å, 55 Å and 75 Å with Al<sub>0.3</sub>Ga<sub>0.7</sub>As barrier layers of 400 Å. Photoluminescence of these MQWs showed clear peaks corresponding to the three quantum wells. We have also now successfully grown InAs quantum dots (QD) on GaAs substrate. The AFM images clearly show growth of quantum dots of different heights, typically less than 10 nm, which lies in the quantum confinement regime. For this end, we have started work on epitaxial growth of (Al<sub>1-y</sub>Ga<sub>y</sub>)<sub>x</sub>In<sub>1-x</sub>P/(Al<sub>1-y</sub>Ga<sub>y</sub>)<sub>x</sub>In<sub>1-x</sub>P/GaAs QW structures. Initial low temperature photoluminescence measurements show peaks correspond to the QW emission. While working on the growth of Al<sub>x</sub>Ga<sub>1-x</sub>As epitaxial layers in the QW structures, we have observed natural superlattice ordering in the material, which is not reported on (100) GaAs grown by this technique (AIP Conference Proceedings 2016, **1728**, 020243). This growth behaviour is further studied by growth of thick Al<sub>x</sub>Ga<sub>1-x</sub>As layer with different composition and their thermal stability using different x-ray techniques, TEM microscopy and photoluminescence. Effect of the superlattice on emission properties of the QW is also being studied in detail. Apart from MOVPE growth, we are also working on ZnO nanowire based dye-sensitized solar cells. As part of different collaboration, we are also working on Ge nanostructure (*Journal of*

*Experimental Nanoscience*, 2014, **9**, 463), growth of ZnSnP<sub>2</sub>, InN nanowire growth and organic-inorganic composite materials.

- **High- $\kappa$  gate dielectric-based metal-oxide-semiconductor (MOS) devices for different applications**

High- $\kappa$ -based dielectric materials are widely studied for their usefulness as alternative gate dielectric to SiO<sub>2</sub>. Leakage current control through the dielectric is a challenge in high- $\kappa$ -based MOS devices. Three issues are to be addressed to improve high- $\kappa$ -based devices namely, (1) the crystallization process of dielectric films; (2) the degradation mechanism of the electrical properties of the MOS device whether it is crystallization or silicate formation or both and (3) the annealing temperature range above which the performance of the device degrades. Further, there are conflicting views on the influence of crystallization on leakage current properties of MOS devices. An attempt has been made here to address the above issues where HfO<sub>2</sub> is considered as the high- $\kappa$  dielectric material. The glass transition temperatures of amorphous HfO<sub>2</sub> and ZrO<sub>2</sub> were identified. The HfO<sub>2</sub> film gets crystalline nature at ~590 °C due to generation of mechanical stress at the interface. Densification of top HfO<sub>2</sub> layer and bottom interfacial SiO<sub>2</sub> swelling upon annealing at higher temperature generate stress and a critical stress for crystallization is achieved beyond the above temperature. Further, HfO<sub>2</sub> crystallization temperature decreases with an increase in Hf content in the HfO<sub>2</sub> film. The effect of lateral distribution on fixed oxide charges in the MOS device is simulated and experimentally verified. The variation of residual stress with deposition and annealing conditions is measured for a < 10 nm-thin HfO<sub>2</sub> film. An equation for estimation of the stress for such a thin-film is also derived and proposed. The crystallization process ZrO<sub>2</sub> thin-film is identified and found that 1-D crystal growth took place initially that spreads laterally with temperature and time without increasing their numbers. The growth of Zr-Silicate and silicide is also investigated using differential scanning calorimetry. The substrate dependent performance of the high- $\kappa$  dielectric film is also investigated. Charge storage properties of InP quantum dots in GaAs metal-oxide-semiconductor based nonvolatile flash memory devices is also investigated. A nanoparticle (NP)-based non-volatile memory devices with HfO<sub>2</sub> as tunnel and barrier layers are fabricated and characterized. The deposited NP sizes and densities, deposited on the tunnel oxide, are independently controlled by using a nano-cluster source coupled with quadrupole mass filter assembly. The memory performance is improved with a reduction in NP size and for an optimum number density.

- **Swelling dynamics of ultrathin polymer films and electronic properties of organic semiconducting ultrathin films**

Structure and swelling dynamics of ultrathin polymer films and polyelectrolytes. The films were prepared from polymer solutions by spin coating technique. The structure and the swelling properties of the films are investigated using AFM and X-ray reflectivity techniques at our laboratory as well as at synchrotron facilities. We have carried out an India France (CEFIPRA) bilateral collaboration in this area of research. I had undertaken several visits to our French collaborator to perform experiments in the French laboratories. We have published several papers in this field. Organic semiconducting (OSc) materials are taking over the conventional semiconductors in many applications day by day. Nano dimensional thin films of small molecules have been the object of much investigation because of potential use in organic electronics and spintronics. We work with nano dimensional OSc thin films prepared on various substrates in ultra high vacuum chamber. Structure and electronic properties of these films are studied. OTFT devices are prepared and the field effect mobility of the devices are measured. We use various spectroscopic and microscopic techniques for our experiments such as XPS/UPS, NEXAFS, PRES (synchrotron based techniques), AFM etc. We also perform density functional theory calculations using StoBe and VASP software. The objective of our study is to understand interfacial properties that are required for the development high mobility organic semiconductor devices.

- **Surface plasmon (SP) enhanced photonics of single metal nanoparticle**

Surface plasmon polaritons (SPP) are electromagnetic (EM) surface waves excited by EM fields, i.e., light or evanescent waves associated with a fast moving electrons to collective oscillations of the conductor's electron. Under resonant excitation, while surface plasmon resonance (SPR) occurs at metal/dielectric interfaces, the same is called as localized surface plasmon resonance (LSPR) occurring at nanometer-sized metallic structures. At resonant wavelength, LSPR decays to enhanced far-field radiation showing highly localized EM field enhancement on the nanoparticle's surface which has several remarkable applications and forms the basis of Plasmonics, a promising branch of nano-photonics research that exploits the unique optical properties of metallic nanostructures to route and manipulate light at nanometre length scales. Detection of electron beam induced radiation emission (EIRE), also called as cathodoluminescence (CL) in a scanning electron microscope (SEM) is shown to constitute an excellent probe of plasmons. In CL-SEM technique, information on the near field electromagnetic (EM) enhancement can be captured through the detection of far field radiation. In addition to acquiring high resolution spectral data we also record maps of spatial variation of photon emission with high spatial resolution in 10-50 nm range in visible wavelength which is regarded as a direct probe of resonant modes of plasmonic nanostructures thus providing a direct way to map the local electric fields. As the electron beam can be raster scanned in SEM, one can also obtain the information about the spatial variations of the EM local density of states (EMLDOS). Experimental data are analysed with FDTD numerical simulation to generate near field intensity maps and electric field vector plots. The methodology discussed in our recent works [J. Phys. Chem. C 2017, **121**, 731; J. Phys. Chem. C 2016, **120**, 27003; ACS Photonics 2014, **1**, 1290; J. Phys. Chem. C 2012, **116**, 15610] is expected to give an alternating pathway to understand the near field-optical properties including tip-to-tip coupling for multibranch / tipped structures, substrate-induced hybridization and existence of higher order plasmonic modes for complex and large metal nanoparticles which may have stronger implications in novel applications, such as in surface-enhanced Raman scattering, catalysis, sensing, and imaging.

- **Gas sensing and Photoacoustic detection**

We have explored the possibility of using low cost room temperature CNT-based gas sensors prepared on plastic substrates to monitor the presence of ammonia in the environment, where NH<sub>3</sub> concentrations in the low-ppb range are expected. The detection of ammonia atmospheric concentrations in urban areas has been so far widely overlooked, since its average levels are usually low, i.e. in the 20-30 ppb range. We prepare a sensing material which operates in the ammonia environment of 1 to 1000 ppb and it recovers in normal air environment without any purging of gas.

The effect of confinement of hemoglobin molecules on photoacoustic (PA) signal is studied experimentally. The PA amplitudes for samples with suspended red blood cells (SRBCs) and hemolyzed red blood cells (HRBCs) were found to be comparable at each hematocrit for 532 nm illumination. The intended application is the noninvasive detection of hemolysis. Hemolysis can be detected visually. Although it is not a very accurate method, it serves as a quick and easy method. The experimental results demonstrate that the PA amplitude for the SRBCs is about 2.6 times greater than that of the HRBCs at 40% hematocrit for 1064 nm irradiation.

- **Nanoscale adhesion and self-organization of molecules in soft membranes**

Adhesion of molecules specifically the biomolecules or nanoparticles in lipid membrane and their migration over and across the membrane initiated by the changes in the environment surrounding the membrane have drawn significant attention in recent days. It is believed that the physical parameters like surface tension, stretching and bending elasticity, viscosity etc. changes dramatically due to the attachment of proteins, ions or nanoparticles with the membranes. So the extraction of these physical parameters in a membrane is very important. X-ray scattering techniques are very useful to give us the information about the buried structure of the molecules in the membranes. Due

to its high brilliance, x-ray synchrotron sources are particularly very helpful as the scattering is very weak from such biomolecules or nanomaterials. In our laboratory in SINP, we have developed a technique to prepare bio-membranes on soft surfaces like polymer brush. We deposit first the polymer brush on solid substrate and then the bio-membranes using Langmuir-Blodgett film deposition technique available in our laboratory. We have studied the adhesion and the interaction of the skeletal proteins in the lipid bilayer membranes using reflectivity and diffuse scattering techniques. The study reveals the interesting observation of formation of skeletal network and brush like network depending on the polar head group size of the bilayer membranes. Similarly, there are other molecules like cholesterol and heme molecules which are very important for the raft like structure formation or toxicity effect in lipid membranes respectively. We study the structures in different phases and their incorporation into the membrane depending on the temperature-surface pressure phase diagram of the mixed lipids. Recently, we have published two papers in *Langmuir* **33**, 1295 (2017) and *J. Phys. Chem B* **121**, 4081 (2017) on these works. Self organization mechanism in supramolecular materials in presence of foreign species is also very crucial in developing new functional devices based on these self assembled materials. In a recently published paper in *Scientific Reports* **7**, 246 (2017), we have demonstrated that these supramolecular nanofibers are very promising candidates for various applications such as solar cells, sensors, FETs, etc. The change in structural arrangements of the nano fibres as a function of humidity using in-situ grazing incidence small angle x-ray scattering (GISAXS) measurements show the aridity dependent self reorganization of the nanofibers.

- **Dynamics in soft materials**

The research under this theme consists of (1) Phase transition in pure and mixed liquid crystals, (2) Long-term dynamics of two-dimensional complex fluids, (3) Evolution of two-dimensional patterns at the nanoscale, and (4) Interaction of drugs with biologically interesting molecules. In the first category we have found that the Nematic-Isotropic phase transition in some liquid crystalline materials is a non-equilibrium transition and can be changed into an equilibrium transition by enthalpic forces. Such liquid crystalline materials serve as reductive-self assembling matrices for one-step fabrication of nanocrystals with tunable morphology. In the second group we have found two important results. We have shown that (a) lipophilic attraction between hydrocarbon chains is the driving force at all stages of long-term monolayer dynamics, and the structures evolving in the monolayers have fractal nature with two fractal dimensions, and that (2) critical behaviour in two-dimensional liquids is preceded by a 'precritical' stage characterized by fluctuations in the order parameter and by unstable domains of fingering or dendritic morphology as well as proliferation of a large number of small sized domains. In the third category the main result is that two-dimensional nanoscale pattern dynamics at air-water interface through de-mixing of Au nanoparticles and fatty acids in a mixed monolayer is completely controlled by lipophilic forces, giving rise to chaotic distributions and dynamics at different timescales. In the final group we have found that (a) drug-DNA interaction in thin films segregates the drug molecules in a top layer of the film, and counterions in buffer enhance this segregation, and (b) drug-lipid interaction in monolayers, serving as the bio-mimic of drug-cell membrane interaction, indicates an optimum drug dose for effective membrane fluidization.

- **Nanostructured electrode materials for bio-sensors and electrochemical capacitors**

The nanomaterial based electrochemical electrodes have caught immense attention because of their potential application as bio-sensors and electrochemical capacitors. Electrochemical electrodes based on nanostructured materials can replace enzyme immobilized electrodes and electrochemical capacitors can be used as electrical energy storage devices which can deliver high power when needed. Non-enzymatic bio-sensing electrode can be reused several times and also for different analytes. Electrochemical capacitors have higher energy density than conventional dielectric capacitors and have shorter charging time and larger cycling life than batteries. Hence,

electrochemical capacitors can fill the gap between batteries and conventional capacitors. We have gain sufficient knowledge on how to choose the appropriate nanostructured electrode materials for both these application (bio-sensor and supercapacitor) leading to notable improvement in device performance. We have also made advances in understanding bio-sensing and charge storage mechanisms and the development in the synthesis of these advanced nanostructured electrode materials based on transition metal oxides and nanostructured graphene.

- **Understanding the origin of magnetism in nano-form of nonmagnetic bulk materials:nano-form of oxides, carbon and metals**

Diamagnetic materials exhibits negative magnetization as a function of applied magnetic field. But, recently we have reported observation of positive magnetization in nano-forms of otherwise some diamagnetic bulk materials. These nano-form of materials ranging from insulating oxides to carbon based semimetals to even good metals like gold exhibited positive magnetization. We have tried to understand the origin of magnetism (positive magnetization) in these nano-form materials. The origin of magnetism in oxides was attributed to presence of oxygen vacancy clusters. We proposed that isolated F<sup>+</sup> centers with spin 1/2 can couple antiferromagnetically with vacancy clusters (superexchange) which can give rise to a ferrimagnet with a net moment and also the delocalization of electrons between unequal size vacancy clusters can give rise to ferromagnetism (double exchange). We have found from quantum chemical calculations using dispersion corrected density functional theory that for carbon based materials such as graphene oxide (GO), upon thermal reduction, the GO sheets starts tearing or cutting from cis-edge (arm-chair) leading to fragments of smaller size graphene sheets exposing predominantly trans (zig-zag) edges. We observe that upon thermal reduction of GO the magnetization of the material increases and we have argued that zig-zag edges play an important role for the observation of positive magnetization in these carbon based materials. Observation of magnetism in nano form of gold could be explained by invoking existence of a contact potential  $V$  and a radial electric field (perpendicular to the interface) giving rise to a Rashba type spin-orbit interaction. All these aspect with proper perspective related to magnetism arising in nano-form is under investigation.

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*Structural and Morphological Evolution in Metal-Organic Films and Multilayers*, Alokmay Datta and Smita Mukherjee, *Taylor and Francis*, 6 October 2015.

## Book Chapters

Sputter-ripple formation on flat and rough surfaces – a case study with Si, SA Mollick and D Ghose in: *Nanofabrication by Ion-Beam Sputtering: Fundamentals and Applications* (Eds.: T Som and D Kanjilal), Pan Stanford Publishing Pte. Ltd., Singapore, 2013. pp. 41 – 71.

## **ALOKMAY DATTA, Sr. Professor H+**

DoB 22 August 1957  
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**EDUCATION** 1989: Ph.D. in Physics, University of Calcutta  
1980: M.Sc. in Physics, University of Calcutta; 2nd class  
1978: B.Sc. Physics Hons, University of Calcutta; 2nd class

**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  
2004-2007: Professor F, Saha Institute of Nuclear Physics  
2000-2004: Associate Professor E, Saha Institute of Nuclear Physics  
1994-2000: Reader D, Saha Institute of Nuclear Physics  
1990-1994: Lecturer C, Saha Institute of Nuclear Physics

**AWARDS/HONOURS** MRSI Medal 2014  
MATISSE Visiting Professor, Université Pierre et Marie Curie, Paris, France, April 2014  
Eminent materials Scientist of the year 2010  
JSPS Visiting Professor, Department of Physics, Kyoto University, Japan, 2008-2009  
National Science Foundation (US) Post Doctoral Fellow, Northwestern University, National Synchrotron Light Source & Advanced Photon Source, USA, 1998-2000  
Fellow, West Bengal Academy of Science and Technology, 2006

**PUBLICATION STATISTICS** Journals: 104 (for 2012-2017: 26); Conference: 70; Chapter of Books: 3; Others: 1  
*h*-index: 22

**SELECTED PUBLICATION** Entropic screening preserves non-equilibrium nature of nematic phase while enthalpic screening destroys it, K. Dan, M. Roy, **A. Datta**, *J. Chem. Phys.* **144**, 064901 (2012-2017) (2016)

Time-structuring in the evolution of 2D nanopatterns through interactions with substrate, M. Choudhuri, **A. Datta**, *Soft Matter* **12**, 5867 (2016)

Critical behavior of a two-dimensional complex fluid: Macroscopic and mesoscopic views, M. Choudhuri, **A. Datta**, *Phys. Rev. E* **93**, 042804 (2016)

Evolution of self-organized two-dimensional patterns of nanoclusters through demixing, M. Choudhuri, A.N. Sekar Iyengar, **A. Datta**, M. S. Janaki, *Phys.Rev. E* **92**, 032907 (2015)

Non-equilibrium phase transitions in a liquid crystal, K. Dan, M. Roy, **A. Datta**, *J. Chem. Phys.* **143**, 094501 (2015)

Stability and softening of a lipid monolayer in the presence of a pain-killer drug, U. K. Basak, **A. Datta**, D. Bhattacharyya, *Colloids and Surfaces B* **132**, 34 (2015)

Atomic force microscopy in biofilm study, S. Chatterjee, N. Biswas, **A. Datta**, R. Dey, P. K Maiti, *Microscopy*, **63**, 269 (2014).

Convex Arrhenius behaviour in a nematic-isotropic phase transition, K. Dan, M. Roy, **A. Datta**, *Europhysics Letters* **108**, 36007 (2014).

Evolution of nanoparticle-induced distortion on viral polyhedra, S. Das, **A. Datta**, S. Mukherjee, N. Biswas, A. Goswami, *Journal of Biological Physics* **39**, 173 (2013).

Nanoparticle-induced morphological transition of Bombyx mori nucleopolyhedrovirus: a novel method to treat silkworm grasserie disease, S. Das, A. Bhattacharya, N. Debnath, **A. Datta**, A. Goswami, *Appl Microbiol Biotechnol* **97**, 6019 (2013).

Phase separation in crowded micro-spheroids: DNA-PEG system, N. Biswas, M. Ichikawa, **A. Datta**, Y. T. Sato, M. Yanagisawa, K. Yoshikawa, *Chem. Phys. Lett.* **539–540**, 157 (2012).

**TEACHING/ GUIDANCE** Ph.D. degree awarded: 8 [in the period 2012-2017: 5]; Thesis submitted: 1

#### **AREA(S) OF RESEARCH:**

- Monomolecular Layers at Water Surface
- Metal-Organic Multilayers
- Polymer Thin Films
- Liquid Crystalline Phases
- Nanocrystal Growth
- Biomaterials and Nano-bio Interactions
- Molecular Spectroscopy and Light-Molecule Interaction
- Structure at Surfaces and Interfaces of Semiconductor Multilayers

#### **ESSENTIAL STRENGTH OF RESEARCH / DEVELOPMENT OUTPUT:**

My research has been focused on soft matter, including liquids, nano-composites and biomaterials, in particular on ultrathin films and their surfaces and interfaces. Till 2010 my contributions were mostly on the structure of such films and the interfaces of organic monolayers with metal ions. The former showed the emergence of spontaneous order even for simple liquids and the consequent breakdown of hydrodynamics, whereas in the latter case the metal ions self-organized into two-dimensional lattices that are dictated by the organic monolayers and can be tuned by external parameters. These works have initiated new research on nanofluids, nano-mineralization, and the role of the metal-organic interface on biomaterials. Since 2010, I have extended the scope of my investigations to the dynamics at these interfaces. In particular, I have started to collaborate with researchers in biosciences and medicine, to understand the dynamics of nanoparticle-induced destruction of the outer membranes of viruses. I have also been able to understand the optimization of drug dosage on the basis of fluidization of the bio-membrane caused by pain-killer drugs. I, with my collaborators, have also made a quantitative estimate of the damage done by antibiotics to bacterial biofilms. On the other hand, I have studied the evolution of two-dimensional patterns of metal nanoclusters on organic monolayers and I am investigating the optical and transport properties of these dendritic patterns, transferred onto suitable substrates, to assess their energy storage efficiency.

#### **FUTURE RESEARCH/DEVELOPMENT PLAN:**

I have now entered into an informal collaboration with the Department of Microbiology, IPGMR, SSKM Hospital, Kolkata, to initiate a rigorous study of the correlation of size and shape of nanoparticles (especially Ag) to their anti-bacterial efficiency, both as a stand alone and as a synergistic agent with standard antibiotics, against persistent antibiotic-resistant bacteria. I am also working informally with faculty members of Calcutta University, West Bengal University of Technology, and Tripura University on the dynamics of biofilm growth and the effect of Ag nanocrystals (grown by methods developed by us) on this growth. My third area of interest will be on the two-dimensional patterns mentioned above.

## Satyanarjan Bhattacharyya, Sr. Professor H

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**EDUCATION** 1993: Ph.D. in Physics, University of Calcutta  
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1980: B.Sc. Physics Hons, University of Calcutta

**ACADEMIC POSITIONS** 2016- ..... : Senior Professor H, Saha Institute of Nuclear Physics  
2009-2016: Professor G, Saha Institute of Nuclear Physics  
2006-2009: Professor F, Saha Institute of Nuclear Physics  
2002-2006: Associate Professor E, Saha Institute of Nuclear Physics  
1998-2002: Reader D, Saha Institute of Nuclear Physics  
1996-1998: Lecturer C, Saha Institute of Nuclear Physics  
1995-1996: Post Doctoral Fellow, Physics Dept., University of Bielefeld, Germany  
1993-1995: Post Doctoral Research Associate, Saha Institute of Nuclear Physics

**AWARDS/HONOURS** Visiting Scientist, Forschungszentrum Jülich, Germany, 2017  
Nominated scientist from India in the INSA-DFG Exchange Programme:  
2010 and 1999, Universität Greifswald, 2005; Hahn-Meitner-Institute; Germany  
Visiting Scientist in Max-Planck Institute for Plasmaphysics, Germany, 2005  
Principal investigator for the project under Indo-Italian Program, 2002.  
Premchand-Raychand Scholarship, University of Calcutta, 1987.

**PUBLICATION STATISTICS** Journal: 74 (for 2012-17: 25), Chapter of book: 1, Conference Proceedings : 15  
h-index 14

**SELECTED PUBLICATION (2012-2017)** Role of oxygen vacancy on the hydrophobic behavior of TiO<sub>2</sub> nanorods on chemically etched Si pyramids, C. P. Saini, A. Barman, D. Das, B. Satpati, **S. R. Bhattacharyya**, D. Kanjilal, A. Ponomaryov, S. Zvyagin and A. Kanjilal, *J. Phys. Chem C* **121**, 278 (2017).  
Defect-engineered optical bandgap in self-assembled TiO<sub>2</sub> nanorods on Si pyramids, C.P. Saini, A. Barman, B. Satpati, **S.R. Bhattacharyya**, D. Kanjilal and A. Kanjilal, *Appl. Phys. Lett.*, 108, 011907 (2016).  
Formation of monodispersed films from size-selected copper nanoclusters, S. Mondal, B. Satpati and **S.R. Bhattacharyya**, *J. Nanosci. Nanotechnol.* 15, 611 (2015).  
Oxidation behaviour of Copper nanofractals produced by soft-landing of size-selected nanoclusters, S. Mondal and **S.R. Bhattacharyya**, *RSC Adv.* 5, 99425 (2015).  
Performance of a size-selected nanocluster deposition facility and in situ characterization of grown films by x-ray photoelectron spectroscopy, S. Mondal and **S.R. Bhattacharyya**, *Rev. Sci. Instrum.* 85, 065109 (2014)  
Morphological and optical properties of soft-landed supported nanoclusters: effect of rapid thermal annealing, S. Mondal, **S.R. Bhattacharyya**, *Appl. Phys. A* 116, 1621 (2014)  
Mechanism of ion induced mixing phenomena in Gold-Nickel bilayer on Si substrate, D. Datta and **S.R. Bhattacharyya**, *Appl. Phys. A* 116, 1455 (2014)  
Wetting and surface energy of vertically aligned silicon nanowires, S. Jana, S. Mondal, **S.R. Bhattacharyy**, *J. Nanosci. Nanotechnol.* 13, 3983 (2013).  
Growth process of GaAs ripples as a function of incident Ar-ion dose, D. Datta, S. Mondal, **S.R. Bhattacharyya**, *Appl. Surf. Sci.* 258, 4152 (2012).

**TEACHING/** Ph.D. awarded: 1, Thesis submitted 1  
**GUIDANCE** Current PhD students: 1

### **AREAS OF RESEARCH**

- Sputtering and Sputter-induced surface morphology including nanopatterning
- Ion beam mixing of metallic thin films
- Swift heavy ion interaction on solid surfaces
- Thin films formation by size-selected nanocluster deposition and their properties

### **ESSENTIAL STRENGTH OF RESEARCH/DEVELOPMENT OUTPUT**

Energy dependence of sputtering yields of GaAs bombarded by mass analysed  $^{40}\text{Ar}^+$ ,  $^{84}\text{Kr}^+$  and  $^{132}\text{Xe}^+$  ions. This work showed that spike effect in sputtering has a projectile dependent component apart from energy dependence as proved for higher masses projectiles. This investigation is considered as one of the pioneering works for spike effect of sputtering for compound semiconductors. (A detailed discussion on this aspect is found in a work by J.B. Malherbe, CRC Crit. Rev. Solid State & Materials Sci. vol. 19(2) (1994) p.55)

Surface morphology studied for metals, semiconductors and insulator (glasses) bombarded by energetic ions (keV range). Cone formation on metals for normal incidence and ripple formation on Si, GaAs and glasses for oblique incidence. Energy dependent wavelength of nanoscale ripples has been predicted. Ion beam mixing and interface alloying of thin films have been studied using medium energy keV ions of inert gases.

Light emission from ion bombarded solid surfaces was studied for metals, semiconductors and insulators. Relative sputtering and desorption yields were measured from Si surfaces under polyatomic and highly charged ions respectively.

Highly charged and high energy (beyond 100 MeV) heavy ions (Xe, Au etc.) interactions on solid surfaces, particularly insulator surfaces (BeO, SiO<sub>2</sub>, SeO, Al<sub>2</sub>O<sub>3</sub> etc.) for studies of hydrogen desorption and Coulomb explosion and related topics for studies of basic mechanism of such kind of interactions.

A new proposal of size-selected nanocluster deposition and characterization was undertaken and was executed in 2010. For this gas aggregation type cluster source with magnetron sputtering unit was procured. For selection of size or mass of a cluster, a quadrupole mass filter with high resolving power and capable of measuring a mass of a cluster with 1000 atoms in the medium z-element was procured. The system is equipped with in-situ XPS for the information of composition as well as chemical states of cluster once deposited on a substrate. This unique gas aggregation type size-selected nanocluster deposition with in-situ XPS facility is the first of its kind in India and has been recognized by the international community of nanoclusters science and technology. As a mark of this recognition, Prof. Bhattacharyya was invited to deliver an invited talk in the *International Workshop of Nanocluster Synthesis, Characterization and Application* held at Okinawa Institute of Science & Technology, Japan, May 16-19, 2016.

### **FUTURE RESEARCH/DEVELOPMENT PLAN**

Size-selected nanocluster deposition on various substrates for applications in solar cell for enhanced efficiency, catalytic behavior of functional thin films composed of size-selected clusters and other properties of these films will be investigated. The possibility of the extension of applications of nanoclusters in other fields like biochemical and biomedical will be explored.

The low energy ion beam facilities including negative ion implanter will be utilized to get functional layers in bulk or thin films for suitable application.



## TAPAS KUMAR CHINI, Professor G

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- EDUCATION** 1994: Ph.D. in Physics, University of Calcutta  
1985: M.Sc. in Physics, University of Calcutta  
1983: B.Sc. Physics Hons, University of Calcutta
- ACADEMIC POSITIONS** 2010- ..... : Professor G, Saha Institute of Nuclear Physics  
2007-2010: Professor F, Saha Institute of Nuclear Physics  
2003-2007: Associate Professor E, Saha Institute of Nuclear Physics  
2000-2003: Reader D, Saha Institute of Nuclear Physics  
1998-2000: Postdoctoral Fellow, Institute of Physics, Bhubaneswar  
1997-1997: Postdoctoral Fellow, University of Houston, USA  
1995-1997: Postdoctoral Fellow, Saha Institute of Nuclear Physics  
1993-1995: Monbusho Scholar, Nagoya Institute of Technology, Nagoya, Japan
- AWARDS/HONOURS** Guest Scientist, Institute of Ion Beam Physics & Materials Research, Germany 2006  
Visiting Scientist, Universidad Carlos III De Madrid, Spain, Nov. 2005  
Awarded AIEJ (Japan) Research, Nagoya Institute of Technology, Nagoya, Japan 2002
- PUBLICATION STATISTICS** Journals: 56 (for 2012-2017: 9)  
Average Impact Factor for 2012-2017: 4.7; Average Citation: 15; *h*-index: 16
- SELECTED PUBLICATION (2012-2017)** Probing higher order surface plasmon modes on individual truncated tetrahedral gold nanoparticle using cathodoluminescence imaging and spectroscopy combined with FDTD simulations, P. Das, **T. K. Chini**, J. Pond, *J. Phys. Chem. C* **116**, 15610 (2012)  
Spectroscopy and Imaging of Plasmonic Modes Over a Single Decahedron Gold Nanoparticle: A Combined Experimental and Numerical Study, P. Das, **T. K. Chini**, *J. Phys. Chem. C* **116**, 25969 (2012)  
Local electron beam excitation and substrate effect on the plasmonic response of single gold nanostars, P. Das, A. Kedia, P. Senthil Kumar, N. Large, **T. K. Chini**, *Nanotechnology* **24**, 405704 (2013)  
Substrate Induced Symmetry Breaking in Penta-twinned Gold Nanorod Probed by Free Electron Impact, P. Das, **T. K. Chini**, *J. Phys. Chem. C* **118**, 26284 (2014)  
Effect of Intertip Coupling on the Plasmonic Behavior of Individual Multitipped Gold Nanoflower, A. Maity, A. Maiti, P. Das, D. Senapati, and **T. K. Chini**, *ACS Photonics* **1**, 1290 (2014)  
Mode Mixing and Substrate Induced Effect on the Plasmonic Properties of an Isolated Decahedral Gold Nanoparticle, A. Maiti, A. Maity, **T. K. Chini**, *J. Phys. Chem. C* **119**, 18537 (2015)  
Probing Localized Surface Plasmons of Trisoctahedral Gold Nanocrystals for Surface Enhanced Raman Scattering, A. Maity, A. Maiti, B. Satpati, A. Patsha, S. Dhara, **T. K. Chini**, *J. Phys. Chem. C* **120**, 27003 (2016)  
On the efficient excitation of higher order modes in the plasmonic response of individual concave gold nanocubes, A. Maiti, A. Maity, B. Satpati, N Large, and **T. K. Chini**, *J. Phys. Chem. C*, **121**, 731 (2017)

**TEACHING/ GUIDANCE** Ph.D. awarded: 2 [in the period 2012-2017: 1]; Current Ph.D. Students: 2

**AREA(S) OF RESEARCH:**

- Probing localized surface plasmon resonance (LSPR) modes and luminescence from nanostructured materials using cathodoluminescence (CL) imaging and spectroscopy within a scanning electron microscope (FEGSEM).
- Seed mediated chemical synthesis of metal nanoparticles relevant to plasmonics/nanophotonics applications.
- Use of finite difference time domain (FDTD) simulation for understanding LSPR induced effects in the metallic nano-antennas.
- Ion beam modification of surfaces including the effect of sputtering and implantation.

**ESSENTIAL STRENGTH OF RESEARCH / DEVELOPMENT OUTPUT:**

Studies on the localized surface plasmon resonance (LSPR) assisted optical properties of single metal nanoparticle are main thrust of our research. At resonant wavelength, LSPR decays to enhanced far-field radiation showing highly localized electromagnetic (EM) field enhancement on the nanoparticle's surface which has several remarkable applications and forms the basis of plasmonics, a promising branch of nano-photonics research that exploits the unique optical properties of metallic nanostructures to route and manipulate light at nanometre length scales. Detection of electron beam induced radiation, called as cathodoluminescence (CL) in a scanning electron microscope (SEM) is shown to constitute an excellent probe of plasmons. **The essential strength of our research concerns that the CL-SEM technique can be regarded as a true single particle spectroscopy tool where one can record wavelength specific maps of spatial variation of photon emission from single nanoparticle with high spatial resolution in 10-50 nm range, apart from obtaining high resolution spectral data. Such monochromatic photon map is regarded as a direct probe of resonant modes of plasmonic nanostructures thus providing a direct way to map the local electric fields. As the electron beam can be raster scanned in SEM, one can also obtain the information about the spatial variations of the EM local density of states (EMLDOS).** Experimental data are analysed with FDTD numerical simulation to generate near field intensity maps and electric field vector plots. **Our research output thus develops a methodology** [J. Phys. Chem. C 2017, **121**, 731; J. Phys. Chem. C 2016, **120**, 27003; ACS Photonics 2014, **1**, 1290; J. Phys. Chem. C 2012, **116**, 15610] **which is expected to give an alternating pathway to understand the near field-optical properties and plasmonic modal distributions through the detection of far field radiation from single metal nanoparticles with varieties of morphological features having stronger implications in novel applications, such as in surface-enhanced Raman scattering, catalysis, sensing, and imaging.**

**FUTURE RESEARCH/DEVELOPMENT PLAN:**

A major limitation in all thin-film solar-cell technologies is that the absorbance of near-bandgap light is small, in particular for the indirect-bandgap semiconductor Si. Therefore, trapping the light inside the thin-film solar cell to increase the absorbance is of major concern. A new method for achieving light trapping in thin-film solar cells is the use of metallic nanostructures that support surface plasmons. The use of resonant plasmon excitation in thin-film solar cells is to take advantage of the strong local field enhancement around the metal nanoparticles to increase absorption in a surrounding semiconductor material. The nanoparticles then act as an effective 'antenna' for the incident sunlight that stores the incident energy in a localized surface plasmon mode. Based on this idea our future plan concerns the studies on the plasmon assisted improved photovoltaic materials followed by cathodoluminescence microscopy characterization.

## **SANGAM BANERJEE, Professor G**

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- EDUCATION** 1993: PhD in Physics, Indian Institute of Science, Bangalore
- ACADEMIC POSITIONS** 2011- ..... : Professor G, Saha Institute of Nuclear Physics  
2007-2011: Professor F, Saha Institute of Nuclear Physics  
2003-2007: Associate Professor E, Saha Institute of Nuclear Physics  
1999-2003: Reader D, Saha Institute of Nuclear Physics  
1997-1999: Lecturer C, Saha Institute of Nuclear Physics  
1996-1997: Visiting Fellow (RA), Pohang Accelerator Lab, Pohang, South Korea  
1994-1996: Research Associate, Saha Institute of Nuclear Physics  
1993-1994: Research Associate, Indian Institute of Science, Bangalore
- AWARDS/HONOURS** CSIR fellowship, STA fellowship, Japan  
Jun. 2000 to Mar. 2001, Visiting Fellow, European (ESQUI) project on microelectronics PEC, Universite du Maine, France  
Jun – Aug 2002, Visiting fellow, European (ESQUI) project on microelectronics, ST Microelectronics, MDM lab. Milano Italy  
Mar. 2004 to Sept. 2005, Deputation, Setting up nano-science laboratory Materials Science Division, IGCAR, Kalpakkam
- PUBLICATION STATISTICS** Journals: 119 (for 2012-2017: 35); Conference: 70; Chapter of Books: 3; Others: 1  
*h*-index: 25; Average citation 21, Invited seminars abroad: 19
- FOR DETAIL PUBLICATION LIST PLEASE VISIT SITES:**  
my google profile:  
<http://scholar.google.co.in/citations?user=hIzN3uUAAAAJ&hl=en>  
my researcherid:  
<http://www.researcherid.com/rid/B-9026-2016>
- TEACHING/GUIDANCE** Ph.D. awarded in the period 2012-2017: 3; Thesis to be submitted: 3; Current Ph.D. student: 2  
Teaching Post MSc – course on advance condensed matter physics
- AREA(S) OF RESEARCH** **Nanostructured electrode materials for bio-sensors and electrochemical capacitors**  
The nanomaterial based electrochemical electrodes have caught immense attention because of their potential application as bio-sensors and electrochemical capacitors. Electrochemical electrodes based on nanostructured materials can replace enzyme immobilized electrodes and electrochemical capacitors can be used as electrical energy storage devices which can deliver high power when needed. Non-enzymatic bio-sensing electrode can be reused several times and also for different analytes. Electrochemical capacitors have higher energy density than conventional dielectric capacitors and have shorter charging time and larger cycling life than batteries.

Hence, electrochemical capacitors can fill the gap between batteries and conventional capacitors. We have gained sufficient knowledge on how to choose the appropriate nanostructured electrode materials for both these applications (bio-sensor and supercapacitor) leading to notable improvement in device performance. We have also made advances in understanding bio-sensing and charge storage mechanisms and the development in the synthesis of these advanced nanostructured electrode materials based on transition metal oxides and nanostructured graphene.

#### **Understanding the origin of magnetism in nano-form of nonmagnetic bulk materials: nano-form of oxides, carbon and metals**

Diamagnetic materials exhibit negative magnetization as a function of applied magnetic field. But, recently we have reported observation of positive magnetization in nano-forms of otherwise some diamagnetic bulk materials. These nano-forms of materials ranging from insulating oxides to carbon-based semimetals to even good metals like gold exhibited positive magnetization. We have tried to understand the origin of magnetism (positive magnetization) in these nano-form materials. The origin of magnetism in oxides was attributed to the presence of oxygen vacancy clusters. We proposed that isolated  $F^+$  centers with spin  $1/2$  can couple antiferromagnetically with vacancy clusters (superexchange) which can give rise to a ferrimagnet with a net moment and also the delocalization of electrons between unequal size vacancy clusters can give rise to ferromagnetism (double exchange). We have found from quantum chemical calculations using dispersion corrected density functional theory that for carbon-based materials such as graphene oxide (GO), upon thermal reduction, the GO sheets start tearing or cutting from cis-edge (arm-chair) leading to fragments of smaller size graphene sheets exposing predominantly trans (zig-zag) edges. We observe that upon thermal reduction of GO the magnetization of the material increases and we have argued that zig-zag edges play an important role for the observation of positive magnetization in these carbon-based materials. Observation of magnetism in nano-form of gold could be explained by invoking the existence of a contact potential  $V$  and a radial electric field (perpendicular to the interface) giving rise to a Rashba type spin-orbit interaction. All these aspects with proper perspective related to magnetism arising in nano-form is under investigation.

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**ACADEMIC POSITIONS** 2011- ..... : Professor G, Saha Institute of Nuclear Physics  
2007-2011: Professor F, Saha Institute of Nuclear Physics  
2003-2007: Associate Professor E, Saha Institute of Nuclear Physics  
2000-2003: Reader D, Saha Institute of Nuclear Physics

**AWARDS/HONOURS** Young Scientist Award, Indian Science Congress Association, 1989  
CSIR Research Associateship, 1991  
Principal investigator of India-Taiwan bilateral project, March 2009 – March 2012  
Co-investigator, Indo-French (IFCPAR) project, Feb. 2010 – Sept 2014.  
3 years honorary membership of American Chemical Society (ACS) since Nov 2015.  
Adjunct Professorship of B R Ambedkar Bihar University, 2015

**PUBLICATION STATISTICS** Journals: 100 (for 2012-2017: 36)  
Average Impact Factor: 2.9; Average Citation: 11; *h*-index: 19

**SELECTED PUBLICATION (2012-2017)** Effect of added salt on swelling dynamics of ultrathin films of strong polyelectrolytes, Tanusree Samanta, Sumona Sinha, **M. Mukherjee**, *Polymer* **97**, 285-294 (2016).  
Study of metal specific interaction, F-LUMO and VL shift to understand interface of CuPc thin films and noble metal surfaces, Sumona Sinha, **M. Mukherjee** *Applied Surface Science* **353**, 540-547 (2015).  
Low-energy positron-nitrogen-molecule scattering: A rovibrational close-coupling study, T. Mukherjee, and **M. Mukherjee** *Phys Rev A* **91**, 062706 (2015).  
Oxidation of Rubrene Thin Films: An Electronic Structure Study, Sumona Sinha, C.-H. Wang, **M. Mukherjee**, T. Mukherjee, Y.-W. Yang, *Langmuir*, **30**, 15433–15441 (2014).  
Swelling dynamics and swelling induced structural changes of polyelectrolyte ultrathin films, Tanusree Samanta, **M Mukherjee**, Andrea Lausi, *Polymer* **55**, 4385–4393 (2014).  
Concentration Mediated Structural Transition of Tri-block Copolymer Ultrathin Films, JK Bal, **M Mukherjee**, N Delorme, MK Sanyal, A Gibaud, *Langmuir* **30**, 5808–5816 (2014).  
Thickness dependent electronic structure and morphology of rubrene thin films on metal, semiconductor, and dielectric substrates, S Sinha, **M Mukherjee**, *Journal of Applied Physics* **114**, 083709 (2013).  
Power law in swelling of ultra-thin polymer films, **M. Mukherjee**, M. S. Chebil, N. Delorme and A. Gibaud, *Polymer* **54**, 4669 (2013).

Crystalline Growth of Rubrene Film Enhanced by Vertical Ordering in Cadmium Arachidate Multilayer Substrate, C. Wang, A. K. M. Maidul Islam, Y. Yang, T. Wu, J. Lue, C. Hsu, S. Sinha and **M. Mukherjee**, *Langmuir* **29**, 3957 (2013).

Effect of thermal modification on swelling dynamics of ultrathin polymer films, M. H. Mondal and **M. Mukherjee**, *Polymer* **53**, 5170 (2012).

Effect of added salt on morphology of ultrathin polyelectrolyte films, T. Samanta and **M. Mukherjee**, *Polymer* **53**, 5393 (2012).

**TEACHING/ GUIDANCE** Ph.D. awarded: 6 [in the period 2012-2017: 4], Thesis to be submitted: 1

#### **AREA(S) OF RESEARCH:**

- Electronic properties of organic semiconducting ultrathin films
- Swelling dynamics of ultrathin polymer films

#### **ESSENTIAL STRENGTH OF RESEARCH / DEVELOPMENT OUTPUT:**

Organic semiconducting (OSc) materials are taking over the conventional semiconductors in many applications day by day. Nano dimensional thin films of small molecules have been the object of much investigation because of potential use in organic electronics and spintronics. We work with nano dimensional OSc thin films prepared on various substrates in ultra high vacuum chamber. Structure and electronic properties of these films are studied. OTFT devices are prepared and the field effect mobility of the devices are measured. We use various spectroscopic and microscopic techniques for our experiments such as XPS/UPS, NEXAFS, PRES (synchrotron based techniques), AFM etc. We also perform density functional theory calculations using StoBe and VASP software. The objective of our study is to understand interfacial properties that are required for the development high mobility organic semiconductor devices. Structure and swelling dynamics of ultrathin polymer films and polyelectrolytes. The films were prepared from polymer solutions by spin coating technique. The structure and the swelling properties of the films are investigated using AFM and X-ray reflectivity techniques at our laboratory as well as at synchrotron facilities. We have carried out an India France (CEFIPRA) bilateral collaboration in this area of research. I had undertaken several visits to our French collaborator to perform experiments in the French laboratories. We have published several papers in this field.

#### **FUTURE RESEARCH/DEVELOPMENT PLAN:**

We plan to continue in the fields of swelling dynamics as well as electronic properties of organic semiconducting films. We have so far performed swelling dynamics in the out of plane direction. Now, we plan to study the dynamics of the films in the in plane direction. The polymer films will be studied using AFM under various humidity condition for this purpose. In the field of electronic properties we will perform XPS, UPS, NEXAFS and RPES studies of the films at our laboratory and synchrotron. The density functional theory (DFT) calculations will be performed using Medea-VASP and StoBe softwares to support our experimental results.

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1990: M.Sc. in Physics, University of Calcutta; 1st class  
1988: B.Sc. Physics Hons, University of Calcutta; 1st class
- ACADEMIC POSITIONS** 2012- ..... : Professor G, Saha Institute of Nuclear Physics  
2007-2012: Professor F, Saha Institute of Nuclear Physics  
2004-2007: Associate Professor E, Saha Institute of Nuclear Physics  
2000-2004: Reader D, Saha Institute of Nuclear Physics  
1998-2000: Postdoctoral Fellow, Universite du Maine, Le Mans, France  
1997-1998: Postdoctoral Fellow, Saha Institute of Nuclear Physics  
1992-1997: Research Fellow, Indian Association for the Cultivation of Science
- AWARDS/HONOURS** PC of BRNS project, 2015-2018; Participant of DST-DAAD project, 2002-2004  
Joint Convener of International Conference SXNS-12 at Kolkata, 2012  
Delegation member, Indo-US Workshop on Nanotechnology, USA, Nov. 2001  
National Merit Scholarship (on the basis of B.Sc. result), University of Calcutta
- PUBLICATION STATISTICS** Journals: 66 (for 2012-2017: 14); Conference: 65; Chapter of Books: 3; Others: 4  
Average Impact Factor: 2.9 (for 2012-2017: 3.1); Average Citation: 18; *h*-index: 19  
[for details see <http://www.saha.ac.in/surf/satyajit.hazra/cite.htm>]
- SELECTED PUBLICATION** Kinetic and isotherm studies on adsorption of toxic pollutants using porous ZnO@SiO<sub>2</sub> monolith, M. Sharma, **S. Hazra** and S. Basu, *J. Colloid Interf. Sci.* **504**, 669 (2017)  
(2012-2017) Structures of spin-coated and annealed monolayer and multilayer poly(3-dodecylthiophene) thin films, I. Roy and **S. Hazra**, *RSC Adv.* **7**, 2563 (2017)  
Growth of thiol-coated Au-nanoparticle Langmuir monolayers through a 2D-network of disk-like islands, M. Mukhopadhyay and **S. Hazra**, *RSC Adv.* **6**, 12326 (2016)  
Solvent dependent ordering of poly(3-dodecylthiophene) in thin films, I. Roy and **S. Hazra**, *Soft Matter* **11**, 3724 (2015)  
Poor solvent and thermal annealing induced ordered crystallites in poly(3-dodecylthiophene) films, I. Roy and **S. Hazra**, *RSC Adv.* **5**, 665 (2015)  
pH-dependent size and structural transition in P123 micelle induced gold nanoparticles, P. Chatterjee and **S. Hazra**, *RSC Adv.* **5**, 69765 (2015)  
Time evolution of a Cl-terminated Si surface at ambient conditions, P. Chatterjee and **S. Hazra**, *J. Phys. Chem. C* **118**, 11350 (2014)  
The hydrophilic/hydrophobic nature of a Cl-terminated Si surface, P. Chatterjee and **S. Hazra**, *Soft Matter* **9**, 9799 (2013)  
Substrate and drying effect in shape and ordering of micelles inside CTAB-silica meso-structured films, P. Chatterjee, **S. Hazra** and H. Amenitsch, *Soft Matter* **8**, 2956 (2012)  
Role of metal ions of LB film in hydrophobic to hydrophilic transition of HF-treated Si surface, J. K. Bal, S. Kundu and **S. Hazra**; *Mater. Chem. Phys.* **134**, 549 (2012)
- TEACHING/GUIDANCE** Ph.D. awarded: 4 [in the period 2012-2017: 3]; Thesis to be submitted: 1

## AREA(S) OF RESEARCH:

**Surface Physics and Low Dimensional systems** with emphasis in understanding:

- the interfacial dynamics and its role in the formation of low dimensional structures
- the controversial nature of Cl-Si surface and its time-evolution from the structure of nanolayers
- the enhancement of preferential ordering of organic semiconductors for better properties
- the self-assembly and 2D-network of nanoparticles
- the growth of nanoparticles from single-step synthesis process

## ESSENTIAL STRENGTH OF RESEARCH / DEVELOPMENT OUTPUT:

It is known that the substrate surface natures (namely, the free energy, the polar/nonpolar or electrostatic nature), initially and after evolution with time, play strong role in the growth and stability/instability of the low dimensional structures (ideal for testing basic physics and have promising applications in different fields) onto it. However, in order to understand the exact role, nondestructive surface/interface sensitive techniques are crucial. **The essential strength of our research is to utilize extensively and successfully two complementary techniques, namely grazing incidence X-ray scattering** (both at laboratory and synchrotron sources) and **scanning probe microscopy** (both at ambient and UHV conditions) **to understand the growth and stability of interesting low dimensional structures and the role of substrate surface/interface on it.** For example, it has been observed that the cylindrical shaped micelles, which are initially circular on a hydrophilic OH-terminated Si substrate in order to form a perfect 2D-hexagonal structure, become elliptical (extended along the in-plane) on a hydrophobic H-terminated Si substrate to form a slightly compressed 2D-hexagonal structure due to a different attachment of the film to the substrate [*Soft Matter* 2012, **8**, 2856]. The Cl-terminated Si surface, which was slightly controversial, was studied and found weak hydrophilic in nature [*Soft Matter* 2013, **9**, 9799]. However, it transforms toward weak-hydrophobic with time due to the growth of less homogeneous oxide layer [*J. Phys. Chem. C* 2014, **118**, 11350]. The crystalline ordering of poly(3-dodecylthiophene) [P3DDT] films, which is of immense importance in their performance as semiconducting materials (as it influence the charge delocalization), is found to depend strongly on the type (viscosity and evaporation rate) of good solvent, both near the film-substrate interface and above it [*Soft Matter* 2015, **11**, 3724] and also on the addition of poor solvent through coil-like to rod-like transition of P3DDT molecules and subsequent  $\pi$ - $\pi$  stacking due to thermal annealing [*RSC Adv.* 2015, **5**, 665]. Formation of 2D-networked structures of disk-like islands for ultrathin Langmuir-Schaefer (LS) films of thiol-coated Au-nanoparticles (DT-AuNPs) on H-passivated Si substrates is evidenced for the first time, directly from a broad peak in grazing incidence small angle X-ray scattering (**GISAXS**) data and also from atomic force microscopy (AFM) images [*RSC Adv.* 2016, **6**, 12326]. The structural information of the LS films, obtained at different surface pressure, helps to infer the growth of Langmuir monolayers of DT-AuNPs, which is very important in understanding the self-assembly process of nanoparticles at the air-water interface and in controlling the growth of 2D-networked nanostructures in large areas.

## FUTURE RESEARCH/DEVELOPMENT PLAN:

Future research plan is to investigate further the **role of interfacial interaction on the growth of low dimensional structures for their better control.** For examples, we want to grow well-covered self-assembled 2D to 3D structures of organic cap metal nanoparticles of tunable size and separation; nanoobjects inside mesoporous structures having controlled size and separation, which will have interesting collective properties. We also plan is to investigate the **role of external forces in the change of conformation of molecules or polymers and their collective shape** by *in-situ* monitor using **complementary techniques** to have a control on them for their use. Further utilizing our **long standing synchrotron experience in GISAXS techniques** (of about 20 years), we want to **develop** a dedicated **SAXS/GISAXS/WAXS laboratory facility**, to determine the morphology of nanostructured and mesostructured films and in some cases their evolution from solution states.



## KRISHNAKUMAR S. R. MENON, Professor G

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**EDUCATION** 1999: Ph.D. in Science, Indian Institute of Science, Bangalore  
1993: M.Sc. in Physics, Indian Institute of Technology, Madras  
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**ACADEMIC POSITIONS** 2016- ..... : Professor G, Saha Institute of Nuclear Physics  
2010-2016: Associate Professor F, Saha Institute of Nuclear Physics  
2007-2010: Associate Professor E, Saha Institute of Nuclear Physics  
2004-2007: Reader D, Saha Institute of Nuclear Physics  
Guest Scientist at Freie University, Berlin, Jan. 2004 – Sep. 2004.  
TRIL Research Fellowship at International Centre for Theoretical Physics (ICTP) and ELETTRA Sincrotrone Trieste, Italy, Jan. 2002 - Dec. 2003.  
Post-Doctoral Associate at Indian Institute of Science, Bangalore, 2001  
NSF Post-Doctoral Research Fellow at University of Connecticut and National Synchrotron Light Source (NSLS), Brookhaven National Laboratory, USA, 2000.

**PUBLICATION STATISTICS** Journals: 54 (for 2012-2017: 23); Conference: 5 (for 2012-2017: 4)

**SELECTED PUBLICATION (2012-2017)** Stabilization of polar  $Mn_3O_4(001)$  film on  $Ag(001)$ : Interplay between kinetic and structural stability, A. K. Kundu, S. Barman and **K. S. R. Menon**, *Surf. Sci.*, Accepted (2017).

Thickness-dependent evolution of structure, electronic structure, and metal-insulator transition in ultrathin  $V_2O_3(0001)$  films on  $Ag(001)$ , A. K. Kundu and **K. S. R. Menon**, *Surf. Sci.*, **659**, 43 (2017).

Microscopic Origin of Colossal Permittivity in Donor- Acceptor (Nb, In) Co-Doped Rutile  $TiO_2$ , S. Mandal, S. Pal, A. K. Kundu, **K. S. R. Menon**, A. Hazarika, Maxime Rioult and Rachid Belkhou, *Appl. Phys. Lett.* **109**, 092906 (2016).

Growth and structural evolution of Sn on  $Ag(001)$ : Epitaxial monolayer to thick alloy film, S. Chakraborty and **K. S. R. Menon**, *J. Vac. Sci. Technol. A* **34**, 041513 (2016).

Growth and characterization of ultrathin epitaxial MnO film on  $Ag(001)$ , A. K. Kundu and **K. S. R. Menon**, *J. Cryst. Growth* **446**, 85 (2016).

A revisit to ultrathin NiO(001) film: LEED and valence band photoemission studies, J. Das and **K. S. R. Menon**, *J. Electron Spectrosc. Relat. Phenom.* **203**, 71 (2015).

Structure of Cr monolayer on  $Ag(001)$ : A buried two-dimensional  $c(2 \times 2)$  antiferromagnet, J. Das, S. Biswas, A. K. Kundu, S. Narasimhan, and **K. S. R. Menon**, *Phys. Rev. B* **91**, 125435 (2015).

Growth of antiferromagnetically ordered Cr monolayer on  $Ag(100)$ , J. Das, A. K. Kundu and **K. S. R. Menon**, *Vacuum* **112**, 5 (2015).

Magnetic skin layer of NiO(100) probed by polarization-dependent spectromicroscopy, S. Mandal, R. Belkhou, F. Maccherozzi, **K. S. R. Menon**, *Appl. Phys. Lett.* **104**, 242414 (2014).

Specular X-ray reflectivity study of interfacial  $SiO_2$  layer in thermally annealed NiO/Si assembly, S. Mitra, S. Chakraborty, **K. S. R. Menon**, *Appl. Phys. A* **117**, 1185 (2014).

Quantum well states in Ag thin films on  $MoS_2(0001)$  surfaces, S. K. Mahatha and **K. S.**

**R. Menon**, *J. Phys.: Condens. Matter* **25**, 115501 (2013).

Electronic structure investigation of MoS<sub>2</sub> and MoSe<sub>2</sub> using angle-resolved photoemission spectroscopy and ab initio band structure studies, S. K. Mahatha, K. D. Patel and **K. S. R. Menon**, *J. Phys.: Condens. Matter* **24**, 475504 (2012).

**TEACHING/** Ph.D. awarded: 4 [in the period 2012-2017: 4]; Thesis submitted: 1  
**GUIDANCE** Current PhD students: 2

#### **AREA(S) OF RESEARCH:**

Electronic structure and magnetism at surfaces, interfaces and ultrathin film; Angle-resolved Photoemission Spectroscopy (ARPES); Synchrotron-based soft X-ray spectroscopies and spectromicroscopies, Growth and structural studies of epitaxial ultrathin films.

#### **RESEARCH & DEVELOPMENT HIGHLIGHTS:**

During the period of 2012 to 2016, the focus of my research has been the **structure-property correlations** at surfaces and ultrathin films of metals, transition metal oxides, metal/semiconductor systems and low-dimensional materials. The different properties include the surface electronic structure and surface/interface magnetism. For surface structure studies, we use Low-energy Electron Diffraction (LEED) and Low-energy Electron Microscopy (LEEM) while the surface electronic structure is investigated using X-ray Photoemission Spectroscopy (XPS) and Angle-resolved Photoemission Spectroscopy (ARPES) and the surface magnetism is probed primarily with synchrotron-based spectroscopic and spectromicroscopic techniques such as X-ray Magnetic Circular Dichroism (XMCD), X-ray Magnetic Linear Dichroism (XMLD) and Photoemission Electron Microscopy (PEEM). By combining these methods as well as other methods, a complete understanding of the material system is achieved together with the Density Functional Theoretical (DFT) calculations. At my laboratory in SINP, we have set up a state-of-the-art ARPES facility where we can perform very high-quality LEED, XPS and ARPES experiments on ultrathin film system which we grow in the growth/preparation chamber attached to the ARPES system.

I have also been actively involved in setting up the SINP Grazing Incidence X-ray Scattering (GIXS) beamline at INDUS-II Synchrotron Centre, RRCAT, Indore along with few other divisional members. The beamline commissioning is in progress and very soon it will be fully operational which will be user facility to perform a verity of experiments such as grazing incidence x-ray scattering studies of surfaces/interfaces in solids and liquids, high resolution X-ray diffraction studies over a wide temperature range (4 K to 1100 K) as well as for *in-situ* growth and characterization of thin films etc. I have also been a part of a team which developed the Indian Beamline at Photon Factory, KEK, Japan which is running very well now which has catered the experimental requirements of many Indian scientists at different institutes and universities.

#### **FUTURE RESEARCH & DEVELOPMENT PLAN:**

Our studies of the electronic structure and magnetism of ultrathin films and surfaces in both laboratory and at different synchrotron facilities shown the absolute necessity to probe the surface at the nanometer scale to obtain a microscopic understanding of the processes occurring at surfaces. In order to achieve this goal of understanding the real-time microscopic dynamical processes occurring at the surfaces of ultrathin films and nanostructured materials with high spatial resolution (<5 nm), a Low-Energy Electron Microscope cum Photoemission Electron Microscope (LEEM-PEEM) facility has been ordered by SINP and is expected to be installed by March 2018. This will be the first LEEM-PEEM facility available in India and can be accessed by all members of SINP as well as users from outside SINP. The availability of this advanced surface microscope will enable us to study the surface structure, morphology, electronic structure and magnetism at the same microscopic region of the sample surfaces with high spatial resolution and will significantly enhance the ability and quality of our research.

## SATYABAN BHUNIA, Associate Professor F

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**EDUCATION** 1999: Ph.D., Indian Institute of Technology, Kharagpur  
1993: M.Sc., Indian Institute of Technology, Kharagpur

**ACADEMIC POSITIONS** 2010- ..... : Associate Professor F, Saha Institute of Nuclear Physics  
2007-2010: Associate Professor E, Saha Institute of Nuclear Physics  
2004-2007: Reader D, Saha Institute of Nuclear Physics  
2003-2004: Assistant Professor in IIT Bombay  
2002-2003: Research Associate, Nippon Telegraph and Telephone Corporation, Japan  
1999-2002: Researcher, The University of Electro-communications, Tokyo, Japan  
1998-1999: Scientist 'B' DRDO, Govt. of India

**SELECTED PUBLICATION (2012-2017)** Phase selective growth of Ge nanocrystalline films by ionized cluster beam deposition technique and photo-oxidation study, S. Mukherjee, A. Pradhan, T. Maitra, S. Mukherjee, A. Nayak, **S. Bhunia**, *Adv. Mater. Lett.* **8** (2017) 891-896.

Pine shaped InN nanostructure growth via vapour transport method by own shadowing and infrared detection, S. M. M. D. Dwivedi, S. Chakrabartty, H. Ghadi, P. Murkute, V. Chavan, S. Chakrabarti, **S. Bhunia**, A. Mondal, *J. Alloy. Compd.* **722** (2017) 872-877.

Investigation of the properties of single-step and double-step grown ZnO nanowires using chemical bath deposition technique, S. Paul, A. Das, M. Palit, **S. Bhunia**, A. Karmakar, S. Chattopadhyay, *Adv. Mater. Lett.* **7** (2016) 610-615.

Mechanochemical devulcanization of natural rubber vulcanizate by dual function disulfide chemicals, S. Ghorai, S. Bhunia, M. Roy, D. De, *Polym. Degrad. Stabil.* **129** (2016) 34-46.

Effect of sol-gel-derived nano-silica on the properties of natural rubber-polybutadiene rubber-reclaim rubber ternary blends-silica nanocomposites", D. De, P.K. Panda, **S. Bhunia**, M. Roy, *Polym.-Plast. Technol. Eng.* **53** (2014) 1131-1141.

Microstructure and dielectric functions of Ge nanocrystals embedded between amorphous Al<sub>2</sub>O<sub>3</sub> films: study of confinement and disorder, A. Nayak, **S. Bhunia**, *J. Exp. Nanosci.* **9** (2014) 463-474.

Synthesis of SiGe layered structure in single crystalline Ge substrate by low energy Si ion implantation, S.A. Mollick, D. Ghose, S.R. Bhattacharyya, **S. Bhunia**, N.R. Ray, M. Ranjan, *Vacuum*, **101** (2014) 387-393.

Reinforcing effect of reclaim rubber on natural rubber/polybutadiene rubber blends, D. De, P. K. Panda, M. Roy, S. Bhunia, *Materials & Design*, **46** (2013) 142-150.

Super rapid response of humidity sensor based on MOCVD grown ZnO nanotips array, P. Biswas, S. Kundu, P. Banerji, **S. Bhunia**, *Sensors and Actuators B-Chemical*, **178** (2013) 331-338.

Reinforcing effect of nanosilica on the properties of natural rubber/reclaimed ground rubber tire vulcanizates, D. De, P. K. Panda, M. Roy, **S. Bhunia**, *Polym. Eng. Sci.*, **53** (2013) 227-237.

**TEACHING/ GUIDANCE** Ph.D. awarded: 1 [in the period 2012-2017: 1]; Thesis to be submitted: 2; Current Ph.D. Students : 2

#### **AREA(S) OF RESEARCH:**

MOVPE growth of compound semiconductor and quantum structures, Electrical and optical properties of semiconductors, High efficiency solar cells, Synchrotron Beamline

#### **Research and Developmental Highlights:**

My overall focus on scientific research during the period of 2012 to 2016 has been in four major areas: 1) Metalorganic Vapour Phase Epitaxial (MOVPE) growth of compound semiconductor and nanostructures, 2) Contribution to development of Synchrotron based material characterization in India, 3) Dye sensitize solar cells fabrication and development using laboratory grown nanomaterial and 4) Collaborative research works

#### **1) Growth and characterization of high efficiency multi-junction solar cell structures using MOCVD**

There is tremendous possibility to achieve very high efficiency solar cells using III-V compound semiconductor materials. High quality epitaxial growth is now the basic technique for growth of AlGaAs/GaAs/Ge and GaInP/GaAs/Ge multi-junction solar cells. The main challenge in realizing such solar cells is the development and understanding of defect-free crystal growth technique of layers of different band gaps which is realized by MOCVD technique. This method provides a good crystal quality of epitaxial structures on Ge substrates, high productivity and reproducibility. Currently, typical multi-junction cells can give efficiency close to 45% and are typically used in strategic applications such as in space and allied areas. There is tremendous scope of further improvement in efficiency by incorporating quantum well and dot structures, increasing the number of the sub-cells etc. This is the high time to target this research in India to match the current scenario and demand in the country.

#### **2) Development of SINP Beamline at INDUS-2 Synchrotron Radiation Facility at RRCAT, Indore**

Our group at SINP has taken full responsibility in developing 'SINP beamline' at INDUS 2 synchrotron radiation facility at RRCAT, Indore. This beamline will be declared as a national facility and would be used for grazing incidence x-ray scattering studies of surfaces and interfaces in solids and liquids, reflectivity, high resolution diffraction studies as a function of temperature, structural & morphological characterization of nanomaterials etc. The entire beamline has been assembled and will be commissioned after some important upgrade process of which is under way. I have taken considerable responsibility in commissioning the Beamline.

#### **3) Dye sensitize solar cells fabrication and development using laboratory grown nanomaterial**

We are continuing research on growth of ZnO nanostructure using the Chemical Vapour Deposition (CVD) technique developed at SINP. We have made a new variant of low temperature CVD technique to grow ZnO nanoflower architectures, which is a hierarchical arrangement of ZnO nanorods. Later on, we have extended this work to fabricate and characterized ZnO nanostructure based dye sensitized solar cells (DSSC). The Dye Sensitized Solar Cells (DSSCs) provide a more effective and inexpensive way to trap sunlight, thereby converting it into electricity.

#### **4) Collaborative research work**

I am engaged with few other other groups such as those from IIT Kharagpur, Presidency University, Kolkata, NIIT Durgapur and MCKV Institute, Kolkata. These collaborative works include growth of Ge nanocrystals and study their properties, growth of ZnSnP<sub>2</sub> as new photovoltaic material, Growth of InN nanowires for photodetector, polymer-inorganic nanocomposites etc.

## MADHUSUDAN ROY, Associate Professor F

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**EDUCATION** 1989: Ph.D. in Physics, North Bengal University  
1983: M.Sc. in Physics, North Bengal University  
1980: B.Sc. in Physics, University of Calcutta

**ACADEMIC POSITIONS** 2012- ..... : Associate Professor F, Saha Institute of Nuclear Physics  
2007-2012: Associate Professor E, Saha Institute of Nuclear Physics  
2002-2007: Reader D, Saha Institute of Nuclear Physics  
1999-2002: Reader, North-Eastern Hill University  
1994:1999: Senior Lecturer, North-Eastern Hill University  
1989-1994: Lecturer, North-Eastern Hill University.  
1988-1989: Research Associate, Indian Association for the Cultivation of Science

**AWARDS/HONOURS** Visiting Scientist Indian Statistical Institute  
Visiting Fellow in Mizoram University  
Guest faculty Vidyasagar

**PUBLICATION STATISTICS** Journal papers: 34 and Conference publications: 8

**SELECTED PUBLICATION** Solid-State Thermal Reaction of a Molecular Material and Solventless Synthesis of Iron Oxide, D. Roy, **M. Roy**, M. Zubko, J. Kusz and A. Bhattacharjee, *Int J Thermophys* (2012-2017) (2016) 37:93,

Mechanochemical devulcanization of natural rubber vulcanizate by dual function disulfide-chemicals, S. Ghorai, S. Bhunia, **M. Roy**, D. De, *Polym. Degrad. Stab.* 129 (2016) 34–46

Entropic screening preserves non-equilibrium nature of nematic phase while enthalpic screening destroys it, K. Dan, **M. Roy**, and A. Datta, *J. Chem. Phys.* **144**, (2016) 064901-1064901-9

Non-equilibrium phase transitions in a liquid crystal, K. Dan, **M. Roy** and A. Datta, *J. Chem. Phys.* **143**, (2015) 09450

Photoacoustic Imaging of Nanoparticle Containing Cells Using Single-Element Focused Transducer: A Simulation Study, S Karmakar, **M. Roy** and R K. Saha, *IEEE Transactions on Ultrasonics, Ferroelectrics, and Frequency Control*, **62(3)**, (2015) 463-474

Positron annihilation study of biopolymer inulin for understanding its structural organization, B Nandi Ganguly, **M. Roy** and S.P. Moulik, *Polymer* **60**, (2015) 137-143

Convex Arrhenius behaviour in a nematic-isotropic phase Transition, K. Dan, **M. Roy** and A. Datta, *EPL*, **108** (2014) 36007-p1- 36007-p5

Magnetic particulate matters in the ashes of few commonly used Indian cigarettes, A. Bhattacharjee, H, Mandal, **M. Roy**, J Kusz and M Zubko, *Environ Monit Assess* , **186(11)** (2014) 7399 -7411

Thermally induced single crystal to single crystal transformation leading to polymorphism, R Saha, S Biswas, S K Dey, A Sen, **M. Roy**, I M Steele, K Dey, A Ghosh,

S Kumar, *Spectrochim Acta A Mol Biomol Spectrosc*, **130** (2014) 526–533

Photoacoustic Response of Suspended and Hemolyzed Red Blood Cells, R. K. Saha, S. Karmakar and **M. Roy**, *Appl. Phys. Lett.* 103, (2013) 044101-1 to 044101-4.

Pressure Effect Studies on the Spin-Transition Behavior of a Dinuclear Iron(II) Compound, A. Bhattacharjee, **M. Roy**, V. Ksenofontov, J. A. Kitchen, S. Brooker, and P. Gutlich, *Eur. J. Inorg. Chem.*, (2013) 843-849

Solventless synthesis of hematite nanoparticles using ferrocene, A. Bhattacharjee, A. Roj, **M. Roy**, J. Kusz, P. Gutlich, *J Mater Sci.*, , **48**, (2013) 2961-2968.

Reinforcing effect of reclaim rubber on natural rubber/polybutadiene rubber blends, D. De, P.K. Panda, **M. Roy**, and S. Bhunia, *Materials and ADesign* **46**, (2013) 142 -150.

Computational investigation on the photoacoustics of malaria infected red blood cells, R. K. Saha, S. Karmakar and **M. Roy**, *PLoS ONE* **7**(12) e51774, (2012) 1-9.;

**TEACHING/ GUIDANCE** Ph.D. awarded in the period 2012-2017: 3; Thesis to be submitted : 3

#### **AREA(S) OF RESEARCH:**

- Gas sensors:
- Photoacoustic detection:

#### **ESSENTIAL STRENGTH OF RESEARCH/DEVELOPMENT OUTPUT**

We have explored the possibility of using low cost room temperature CNT-based gas sensors prepared on plastic substrates to monitor the presence of ammonia in the environment, where NH<sub>3</sub> concentrations in the low-ppb range are expected. The detection of ammonia atmospheric concentrations in urban areas has been so far widely overlooked, since its average levels are usually low, i.e. in the 20-30 ppb range. We prepare a sensing material which operates in the ammonia environment of 1 ppb to 1000 ppb and it recovers in normal air environment without any purging of gas.

The effect of confinement of hemoglobin molecules on photoacoustic (PA) signal is studied experimentally. The PA amplitudes for samples with suspended red blood cells (SRBCs) and hemolyzed red blood cells (HRBCs) were found to be comparable at each hematocrit for 532 nm illumination. The intended application is the noninvasive detection of hemolysis. Hemolysis can be detected visually. Although it is not a very accurate method, it serves as a quick and easy method. The experimental results demonstrate that the PA amplitude for the SRBCs is about 2.6 times greater than that of the HRBCs at 40% hematocrit for 1064 nm irradiation.

#### **FUTURE RESEARCH PLAN**

CMUT fabrication and Harvesting of natural energy: Conceptualisation of roadmap

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**ACADEMIC POSITIONS** 2014- ..... : Associate Professor F, Saha Institute of Nuclear Physics  
2007-2014: Associate Professor E, Saha Institute of Nuclear Physics  
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2002-2003: Microelectronics Division, School of Electrical and Electronic Engineering, Nanyang Technological University, 50, Nanyang Avenue, Singapore 639798  
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1999-2001: Research Assistant – II & I, Department of Electrical and Electronic Engineering, The University of Hong Kong, Pok ful lam Road, Hong Kong  
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1996-1996: Research Student, Electrical Engg. Department, Tokyo Denki University, 2-2 Kanda-Nishiki-cho, Chiyoda-ku, Tokyo 101-8457, Japan  
1991-1996: Research Fellow, Kalyani University

**PUBLICATION STATISTICS** Journals: 35 (for 2012-2017: 17)

**SELECTED PUBLICATION** Interface studies on high-k/GaAs MOS capacitors by deep level transient spectroscopy, S. Kundu, Y. Anitha, **S. Chakraborty** and P. Banerji, *J. Vac. Sci. Technol.*, **30**, 051206 (2012).

Studies on resistive switching characteristics of aluminum/graphene oxide/semiconductor nonvolatile memory cells, S. M. Jilani, T. D. Gamot, P. Banerji and **S. Chakraborty**, *Carbon*, **64**, 187–196 (2013).

Effect of thermal annealing and oxygen partial pressure on the swelling of HfO<sub>2</sub>/SiO<sub>2</sub>/Si MOS structure grown by rf sputtering: a synchrotron reflectivity study, Debaleen Biswas, Sk Abdul Kader Md Faruque, Anil Kumar Sinha, Anuj Upadhyay and **Supratic Chakraborty**, *Applied Physics Letters*, **105**, 113511 (2014).

Development of a linear temperature ramp-based automated system for furnace oxidation of semiconductor wafers, Sk Abdul Kader Md Faruque, Debaleen Biswas, Shaibal Saha and Supratic Chakraborty, *Int. J. Instrumentation Technology*, **1**, 259 (2015)

Study of temperature dependent zirconium silicide phases in Zr/Si structure by differential scanning calorimetry, Sk Abdul Kader Md Faruque<sup>1</sup>, Satya Ranjan Bhattacharyya, Anil Kumar Sinha and **Supratic Chakraborty**, *J. Phys. D: Appl. Phys.*, **49**, 065102 (2016)

Size and density controlled Ag nanocluster embedded MOS structure for memory applications, Debaleen Biswas, Shyamal Mondal, Abhishek Rakshita, Arijit Bose, Satyaranjan Bhattacharyya and **Supratic Chakraborty**, *Materials Science in Semiconductor Processing* **63**, 1–5 (2017).

Crystal growth kinetics of ultra-thin ZrO<sub>2</sub> film on Si by differential scanning calorimetry, Sk Abdul Kader Md Faruque, Debika Debnath, Bimalesh Giri, **Supratic Chakraborty**, *Journal of Crystal Growth* **459**, 38–42 (2017).

Control of interfacial layer growth during deposition of high-κ oxide thin films in reactive RF-sputtering system, Abhishek Rakshit, Arijit Bose, Debaleen Biswas, Madhusudan Roy, Radhaballabh Bhar and **Supratic Chakraborty**, *Applied Surface Science* (2017) <https://doi.org/10.1016/j.apsusc.2017.06.293>

**TEACHING/  
GUIDANCE**      PhD awarded: 1, Thesis submitted: 1, Current Ph. D. Students: 1

#### **RESEARCH INTERESTS:**

Metal oxide semiconductor-based devices (MOS, MOSFETs), High-k dielectric materials, thin-film humidity and gas sensors.

#### **DEVELOPMENTAL ACTIVITIES:**

I along with Prof. Madhusudan Roy proposed, initiated and developed semiconductor grade clean room facilities of Class 100 and 1000 grades in the Institute. The activity begins in 2006 and ended in January 31, 2013.

#### **OTHER INFORMATION:**

Very recently (Dec., 2016), I have joined in the 'Coating group' of LIGO-India collaboration project. The responsibility is to identify appropriate material and technology to grow/deposit material(s) of high mechanical Q (>4000) and their process optimization.



## BISWARUP SATPATI, Scientist F

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**EDUCATION** 2006: Ph.D. in Science, Utkal University  
1997: M.Sc. in Physics, University of Burdwan; 1st class  
1995: B.Sc. Physics Hons, University of Burdwan; 1st class

**ACADEMIC POSITIONS** 2016- ..... : Scientist F, Saha Institute of Nuclear Physics  
2010-2016: Scientist E, Saha Institute of Nuclear Physics  
2009-2010: Scientist C, Central Mechanical Engineering Research Institute, Durgapur  
2007-2009: Scientist C, Institute of Minerals & Materials Technology, Bhubaneswar  
2007-2007: Visiting Scientist, Institute of Physics, Bhubaneswar  
2005-2007: Postdoctoral Fellow, Paul-Drude Institute, Berlin, Germany  
1999-2005: Research Fellow, Institute of Physics, Bhubaneswar

**AWARDS/ HONOURS** MRSI Medal, 2017  
L. K. Panda award, Institute of Physics (IOP), Bhubaneswar, India, 2000

**PUBLICATION STATISTICS** Journals: 232 (for 2012-2017: 150); Conference: 20, Total citation: > 4100  
Av. Impact Factor: >3 (for 2012-2017: >4); Average Citation: >15; *h*-index: 31

**SELECTED PUBLICATION (2012-2017)** Role of oxygen in wetting of copper nanoparticles on silicon surfaces at elevated temperature, T. Ghosh and **B. Satpati**, *Beilstein J. Nanotechnol.*, 8, 425 (2017).  
Study of Gallium Oxide Nanoparticles Conjugated with  $\beta$ -cyclodextrin -An Application to Combat Cancer, B. N. Ganguly, V. Verma, D. Chatterjee, **B. Satpati**, S. Debnath, and P. Saha, *ACS Appl. Mater. Interfaces*, 8, 17127 (2016).  
A high-temperature ferromagnetic topological insulating phase by proximity coupling, F. Katmis, V. Lauter, F. S. Nogueira, B. A. Assaf, M. E. Jamer, P. Wei, **B. Satpati**, et al, *NATURE*, 533, 513 (2016).  
Electrochemical Ostwald Ripening and Surface Diffusion in Galvanic Displacement Reaction: Control over Particle Growth, T. Ghosh, P. Karmakar and **B. Satpati**, *RSC Adv.*, 5, 94380 (2015).  
Study of inelastic mean free path of metal nanostructures using energy filtered transmission electron microscopy imaging, T. Ghosh, M. Bardhan, M. Bhattacharya, and **B. Satpati**, *Journal of Microscopy*, 258, 253 (2015).  
Tilt Boundaries Induced Heteroepitaxy for Chemically Grown Dendritic Silver Nanostructures on Germanium and Their Optical Properties, T. Ghosh, P. Das, T. K. Chini, T. Ghosh and **B. Satpati**, *Phys. Chem. Chem. Phys.*, 16, 16730 (2014).  
Site Specific Isolated Nanostructure Array Formation on a Large Area by Broad Ion Beam without any Mask and Resist, P. Karmakar and **B. Satpati**, *Appl. Phys. Lett.* 104, 231601 (2014).  
Characterization of Bimetallic Core-Shell Nanorings Synthesized via Ascorbic Acid Controlled Galvanic Displacement followed by Epitaxial Growth, T. Ghosh, **B. Satpati** and D. Senapati, *J. Mater. Chem. C*, 2, 2439 (2014).  
Direct Experimental Evidence of Nucleation and Kinetics Driven Two Dimensional Growth of Core-Shell Structures, T. Ghosh, **B. Satpati**, *J. Phys. Chem. C*, 117, 10825 (2013).

**TEACHING/ GUIDANCE** Ph.D. awarded: 1 [in the period 2012-2017: 1]; Current PhD students: 3

### **AREAS (s) OF RESEARCH**

Growth of different low dimensional anisotropic nanostructures in chemical synthesis;  
Interaction of energetic ions with solids (Nanoparticle);  
Nanopatterning; Scanning/Transmission Electron Microscopy (S/TEM).

### **ESSENTIAL STRENGTH OF RESEARCH / DEVELOPMENT OUTPUT:**

The thrust in our research during last 5 years has been to explore a few important issues that are related to growth, structural and optical properties of noble metal nanostructures synthesized *via* chemical routes. These nanomaterials have been characterized extensively by a modern state-of-the-art 300 kV transmission electron microscope (TEM) equipped with associated analytical techniques. The central motivation of our present works is to understand the role of structural parameters, such as crystal orientation, crystal defects/strain on the growth mechanism of the nanoparticles as well as layer structures. With the help of crystallographic relationship between the nucleation centre and the finally grown nanostructure, we have been able to elucidate the growth mechanism of nanoparticles with various morphologies [JPCC 2013, **117**, 10825] and that can be taken as a general growth mechanism to explain the formation of triangular Au, Ag or combined Au-Ag core-shell nanoprisms and nanorods, etc. Our in-depth structural characterization has revealed the crucial role of ascorbic acid towards the fabrication of continuous bimetallic nanorings grown at room temperature [JMCC 2014, **2**, 2439]. Moreover, we have demonstrated a new type of heteroepitaxy [PCCP 2014, **16**, 16730] during the investigation of growth process of Ag nano-inukshuk structures on germanium surface, where the large lattice mismatch between epilayer (silver) and substrate (germanium) is accommodated at the interface by the formation of low-energy asymmetric tilt boundaries. The phenomenon of tilted heteroepitaxial growth as observed in the present analysis is remarkable. It violates our general wisdom on the basic mechanism of the solid state growth process. That an atomically sharp interface (revealed by cross-sectional TEM) plays a crucial role in determining the quality of the cutting-edge new materials having possible applications in next generation electronic, spintronic and quantum computation devices, has recently been demonstrated in a high-temperature ferromagnetic topological insulator utilizing our TEM facility through an international collaborative work [*Nature*, 2016, **533**, 513]. Our TEM work has been instrumental in the discovery of a super dense nonmagnetic fcc phase of cobalt [*Scientific Reports* 2017, **7**, 41856].

### **FUTURE RESEARCH/DEVELOPMENT PLAN:**

Photocatalysts convert solar energy into chemical energy to produce solar fuels or to remove pollutants. Metal oxide semiconductors are extensively used as photocatalysts. However, many metal oxides have a wide band gap, which limits their light absorption to a small spectral region. For example, TiO<sub>2</sub>, which is the most common photocatalyst, only absorbs the ultraviolet light that accounts for less than 5% of all solar radiation. Organic dye molecules and inorganic quantum dots (QDs) have been used as “photosensitizers” to extend the light absorption spectrum of semiconductors to enable the photocatalytic activity at longer wavelengths. Unfortunately, there is some concern about their instability. An alternative to QDs and dye sensitizers is the use of plasmonic metal nanostructures combined with the metal oxide semiconductors to form plasmonic photocatalysts that utilize the plasmonic nanostructure as the sensitizer for semiconductor catalyst. In this project we will do integration of noble metals (*e.g.*, Au, Ag) core and metal oxides (*e.g.*, Cu<sub>2</sub>O, SnO<sub>2</sub>, TiO<sub>2</sub>) shell into single nanostructures for plasmonic enhancement of visible-light photocatalytic activity and structural characterization using TEM. The entire visible-light spectrum will be enhanced by tuning the shell thickness.

## **Mrinmay K. Mukhopadhyay, Associate Professor E**

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**EDUCATIONS** 2005: Ph.D. in Physics, University of Calcutta  
1998: M.Sc. in Physics, University of Calcutta; 1st class  
1996: B.Sc. Physics Hons, University of Calcutta; 1st class

**ACADEMIC POSITIONS** 2011- ..... : Associate Professor E, Saha Institute of Nuclear Physics  
2009-2011: Postdoctoral Fellow, Saha Institute of Nuclear Physics and in-charge of Indian Beamline at Photon Factory, KEK, Japan  
2006-2009: Postdoctoral Fellow, University of California, San Diego and resident user at Advanced Photon Source, Argonne, USA  
1999-2005: Research Fellow, Saha Institute of Nuclear Physics

**PUBLICATION STATISTICS** Journals: 24 (for 2012-2017: 6); Conference: 6 (for 2012-2017: 1)  
*h*-index: 9

**SELECTED PUBLICATION** Dewetting in immiscible polymer bilayer films, J. Lal, S. Malkova, **M. K. Mukhopadhyay**, S. Narayanan, A. Fluerasu, S. B. Darling, L. B. Lurio, and M. Sutton, (2012-2017) *Phys Rev Materials* **1**, 015601 (2017).

Cholesterol-Induced Structural Changes in Saturated Phospholipid Model Membranes Revealed through X- ray Scattering Technique, R. P. Giri, A. Chakrabarti, and **M. K. Mukhopadhyay**, *J. Phys. Chem B* **121**, 4081 (2017).

In-Situ GISAXS Study of Supramolecular Nanofibers having Ultrafast Humidity Sensitivity, A. Bhattacharyya, M. K. Sanyal, U. Mogera, S. J. George, **M. K. Mukhopadhyay**, S. Maiti and G. U. Kulkarni, *Scientific Reports* **7**, 246 (2017).

X- ray Reflectivity Study of the Interaction of an Imidazolium-Based Ionic Liquid with a Soft Supported Lipid Membrane, G. Bhattacharya, R. P. Giri, H. Saxena, V. V. Agrawal, A. Gupta, **M. K. Mukhopadhyay**, and S. K. Ghosh, *Langmuir* **33**, 1295 (2017).

Counterion effects on nano-confined metal-drug-DNA complexes, N. Biswas, S. Chakraborty, A. Datta, M. Sarkar, **M. K. Mukhopadhyay**, M. K. Bera, H. Seto, *Beilstein J. Nanotechnology*, **7**, 62 (2016)

Variation in glass transition temperature of polymer nanocomposite films driven by morphological transitions, S. Chandran, J. K. Basu and **M. K. Mukhopadhyay**, *J. Chem. Phys.* **138**, 014902 (2013)

**TEACHING/ GUIDANCE** Current Ph D Student: 1; Thesis to be submitted: 1

### **RESEARCH INTERESTS:**

#### **(1) Investigation of lipid protein interaction in a membrane:**

The lipid membranes and their interactions with the integral or peripheral protein serve as one of the key mechanism in various cellular functions like communication, cell defences, signal transduction etc. It is believed that the physical parameters like surface tension, stretching and bending elasticity, viscosity etc. changes due to the attachment of proteins/ions with the membranes. So the extraction of these physical parameters from the experiments in a protein conjugated (both integral and

membrane) lipid bilayer is very important. My research interest is strongly related to these activities. We are trying to mimic the cell membrane and then study the structure, interactions and possibly predict the mechanism of various cell functions. For that purpose we have developed a mechanism to prepare a polymer cushioned substrates and deposited lipid bilayer membranes on these soft surfaces. We also study the single monolayer of lipids on water surface that mimics one leaflet of the bilayer membrane and can predict some features observed in cell membranes. A combination of experiments using laboratory x-ray setup, surface pressure – area isotherm measurements from the monolayer and synchrotron x-rays are being used to understand the structure of this assembly and predict the mechanism.

### **(2) Self-assembly of macromolecules in ordered array:**

The self-assembly of polymers or nanocrystals which forms various shapes and sizes by self-assembly are very interesting because of its widespread technological applications in micro- and optoelectronics, optical and protective coatings, adhesives, superhydrophobic and other engineered surfaces, microfluidics, and microreactors. We are studying experimentally the evolution of nano-sized droplet formation as an alternative to these methods in a bottom-up approach by self-organized dewetting of these polymer films. The time dependent GISAXS measurements as the polymer dewets to form various regular structures reveals the growth dynamics of this assembly.

### **(3) Structural transition from 1D structure to 2D and subsequently 3D organization:**

The structural transition of 1D materials, like nanorods or nanowires to make 2D nanosheets has the potential in various applications and here we are trying to make ordered array of such nano-rods or wires by confining them at the air-water interface. The structural transition at the interface as a function of surface pressures and temperature are being observed using GISAXS in the x-ray synchrotron sources. In case of PbS nanorods we observed that they first align perpendicular to the direction of compression and forms long wires on the water surface. At certain temperature these rods join together to make 2 dimensional sheets which ultimately make three dimensional structures upon further compression.

### **(4) Setting up High resolution x-ray scattering instrument at the laboratory in SINP**

I have recently installed a high resolution x-ray scattering setup for reflectivity and diffraction experiments. The instrument has two x-ray tube sources, one Cu K $\alpha$  and the other Mo K $\alpha$  which allows us to even measure the reflectivity from the bilayer samples under water. Normally, the high energy x-ray reflectivity is only available in the various synchrotrons but with the installation of this reflectivity facility now a lot of experiments can be done in SINP laboratory. This is a unique setup in India and the instrument is now being routinely used in SINP laboratory.

### **(5) Development of Indian Beamline at Photon Factory, KEK, Japan.**

I am continuing the development work at the Indian Beamline at Photon Factory, KEK, Japan. The reflectivity from thin films on solid supported substrates and powder diffraction at room temperature and low temperature range was successfully installed during my postdoctoral tenure at the beamline. After that we have added three major facilities in the beamline, (i) liquid surface x-ray scattering facility and (ii) the small angle x-ray scattering facility and (iii) high pressure powder diffraction facility at the beamline. These three facilities are the major upgradation of the beamline and I took the main role in implementing these facilities in this period. The development and realization of various facilities in the Indian Beamline, PF was a major job to me during last few years and successful operation of this beamline with all the facilities is one major achievement in my research carrier.

### **(6) Development of SINP beamline at INDUS II, RRCAT, Indore.**

We are also working for the commissioning part of the grazing incidence x-ray scattering beamline at Indus-II, RRCAT, Indore. Currently we are aligning the various optical components in the beamline. I am expecting to make this beamline operational soon.