



SATYENDRA NATH BOSE NATIONAL CENTRE FOR BASIC SCIENCES



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Editorial

We are happy to bring out the first issue of volume 6. This reflects five consecutive years of successful publication of the S. N. Bose Newsletter. We shall take this opportunity to thank all the members of the Centre, without whose support this would not have been possible. We are sorry that this issue got some what delayed. In fact it turns out that the current schedule of the publication clashes with the interview procedure of the student admission and the Autumn festival. So, it may be useful to consider rescheduling of the publication in future.

The most important event that took place during this period is students' admission. Every academic year the S. N. Bose Centre takes in students for Integrated PhD Programme after their Bachelor's Degree and students for PhD Programme after their Master's Degree. The integrated PhD students take up research works in different departments for their PhD Degree after successful completion of their Master's Degree in the Centre. This year the number of Integrated PhD students who joined the Centre is ten. The admission of students for PhD Programmes is department specific. This year total seventeen students were taken in with the following division among the departments:

Astrophysics & Cosmology – 1, Chemical, Biological & Macromolecular Sciences – 5, Condensed Matter Physics & Material Sciences – 8 and Theoretical Sciences – 3.

The scientific activities of the Centre by such students are reflected by a very large number of high quality theses submitted. The current issue highlights a lot of theses submitted by the students of the Centre.

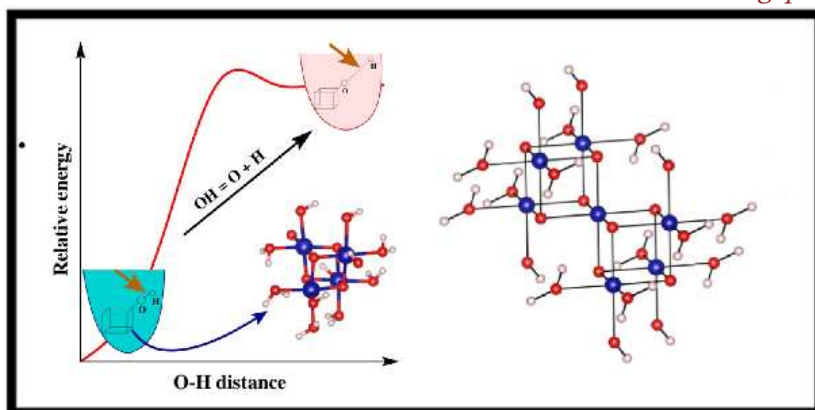
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ACADEMIC REPORT

The role of an oxometallic complex in OH dissociation during water oxidation: a microscopic insight from DFT study

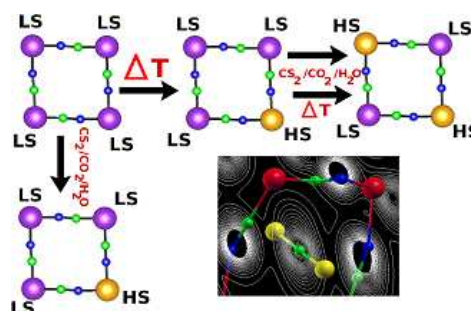
Tanusri Saha Dasgupta



The uncatalyzed atomic dissociation of water requires breaking of a strong O–H bond with an enthalpy of 494 kJ mol^{-1} , which necessitates the understanding and designing of appropriate catalysts. Here we employ transition state theory within quantum chemical density functional theory to understand the role of metal-oxide inorganic complexes in the $\text{OH} \rightarrow \text{O} + \text{H}$ process, the most important reaction in water oxidation. For details see, Soumyajit Sarkar, Mukul Kabir, Martha Greenblatt and Tanusri Saha-Dasgupta, *J. Mater. Chem. A*, 2013, 1, 10422-10428

Two-step spin-switchable tetra-nuclear Fe(II) molecular solid: Ab initio theory and predictions

Tanusri Saha Dasgupta



Using density functional theory supplemented with on-site Coulomb U interaction in combination with ab initio molecular dynamics simulations, we investigate the spin-crossover (SCO) properties of a Fe(II) based cyanide-bridged square molecular system. Our theoretical study predicts further chemo-switching of the spin state by introduction of guest molecules like CO_2 , CS_2 and H_2O into the

porous topology of the system, which would add another dimensionality to this interesting material. For details see, Pablo Maldonado, Sudipta Kanungo, Tanusri Saha-Dasgupta, Peter M. Oppeneer, Phys. Rev. B (Rapid Commun) 2013, **88**, 020408.

Magnonic Band Engineering by Intrinsic and Extrinsic Mirror Symmetry Breaking in Antidot Spin-Wave Waveguides

Dheeraj Kumar and Anjan Barman

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

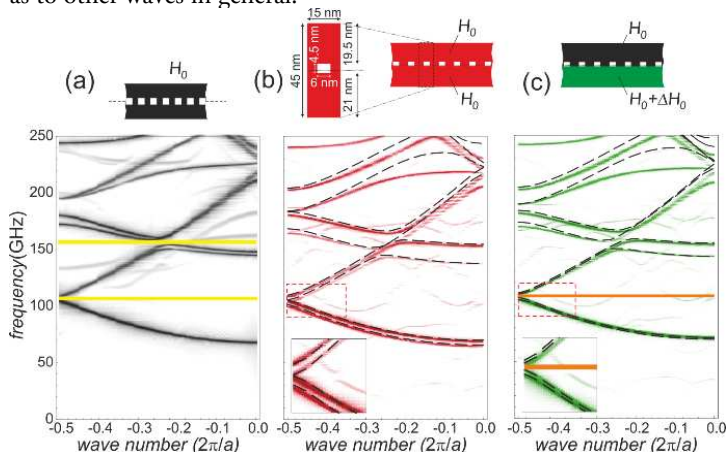


Fig. 1. Magnonic band structures of ADLWs (shown in insets above the main figures where the thin dashed lines mark the mirror plane) calculated with OOMMF (solid lines) and PWM (dashed lines). A part of the 3 nm thick waveguide is shown above (b). Hole size of 6 nm × 6 nm in (a) is changed to 6 nm × 4.5 nm in (b) and (c). Additional bias of $m_0DH_0 = 0.2$ T is applied to the lower sub-waveguide in (c), while $m_0DH_0 = 1$ T is used elsewhere.

The waveguide geometry which was considered for the sample problem is shown above in Figure 1 (b). A bias of 1 T is used along the waveguide in most cases. Figure 1 (a) shows the spin wave dispersion for the case when the waveguide has its mirror symmetry intact the holes are of size 6 nm × 6 nm. Two bandgaps can be seen here. The first (lower frequency stop band) occurs at the Brillouin Zone (BZ) boundary due to the anti-crossing of a pair of degenerate symmetric and anti-symmetric modes. The degeneracy here is a direct consequence of pinning at the ferromagnet/air interface at the waveguide edges and the antidots. The second bandgap opens within the BZ due to anti-crossing of a pair of modes with different number of nodal lines originating in neighbouring BZs. In Fig. 1 (b) we show how the change of hole size to 6 nm × 4.5 nm can affect the collapse of the original bandgaps seen in Fig. 1 (a). We theorized that the change in shape of the dots caused a loss of mirror symmetry of the waveguide; thus, prohibiting any degeneracy of lower modes of spin-wave dispersion. When these modes were forced to move

(due to the loss of the degeneracy), the bandgaps were closed. We further investigated if this collapse of the bandgaps due to an intrinsic (geometrical) factor can be compensated with an extrinsic one like an asymmetric field. We discovered that this was indeed possible and also worked out an analytic expression describing relation between the change in width of the sub-waveguides and the additional bias field that will be needed to restore a bandgap selectively. In Fig. 1 (c) we show the same where an additional bias of 0.2 T has been applied in the wider sub-waveguide to partially recover the first bandgap.

The development of the analytical model presented here was made possible solely by dint of the fundamental properties of discrete translational and mirror symmetries of a crystal lattice. Thus, the main conclusions should not be limited to the particular cases investigated here and it should be possible to extend this idea to other SW waveguides, including those with larger dimensions, or to other types of waves. In the former case the inhomogeneous demagnetizing field, anisotropy of magnetostatic SW dispersion relation, and multimode character of waveguides have to be taken into account. Thus, further investigation is necessary. The compensation effects proposed here should find applications also in other systems, like electrons propagating in a periodically patterned graphene nano-ribbon by the external electric field, or in photonic, plasmonic and phononic waveguides although with tailored electric and elasticity fields, respectively.

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- [1] J. W. Klos, D. Kumar, M. Krawczyk, and A. Barman, *Scientific Reports* 3, 2444 (2013).

FROM THE DEAN (ACADEMIC PROGRAMME)'S DESK

(A) Ph.D. Degree Awardees for the period of May to August 2013

1. Title: Theoretical Studies on the Nonadiabatic effects in Molecular Aggregates by Kinshuk Banerjee; Supervisor: Gautam Gangopadhyay at University of Calcutta on 17.05.2013.
2. Title: Study of Electronic Structure of Disordered Systems by Prashant Singh; Supervisor: Abhijit Mookerjee at University of Calcutta on 07.06.2013.
3. Title: Stochastic approaches to heterogeneous and complex reaction kinetics by Biswajit Das; Supervisor: Gautam Gangopadhyay at University of Calcutta on 24.06.2013.
4. Title: Numerical Simulation of Viscous Accretion Flows Around Black Holes which include Shocks by Kinsuk Giri; Supervisor: Sandip K Chakrabarti at Jadavpur University on 27.06.2013.
5. Title: Heat Transport and Related Thermal Properties in Nanofluids and Nanostructured Materials by Rajesh Kumar Neogy; Supervisor: Arup K Raychaudhuri at Jadavpur University on 27.06.2013.
6. Title: First Principles Study of Silicate Minerals by Swastika Chatterjee; Supervisor: Tanusri Saha Dasgupta at University of Calcutta on 02.08.2013.
7. Title: Heat Pairing and Condensation in Ultracold Quantum Gases by Raka Dasgupta; Supervisor: Jayanta K Bhattacharjee at Jadavpur University on 27.06.2013.

(B) Placement Information

Dr. Hemant Kumar Kashyap has got the placement recently in IIT-Delhi as an Assistant Professor.

THESIS REPORT

Some Applications of Quantum Entanglement

Tanumoy Pramanik

Supervisor: Prof. Archan S Majumdar, Dept. of Astrophysics and Cosmology

The presence of non-local correlation in quantum mechanics gives greater advantages in the information processing tasks over classical theory. This thesis is devoted to study the non-local feature of quantum mechanics and its application in different information processing tasks. In the second chapter, we propose an experimental scheme to show the presence of non-locality at the single particle level. Next, we use the non-local correlation between different degrees of freedom of a single particle to send an unknown quantum state at a distance location, securely. In the chapter-4 and the chapter-5, we study the winning probability of two different quantum games over all possible classical strategy and quantum strategy. In the chapter-4, we show the winning probability of special kind of non-local retrieval games are different when the players use classical correlation, quantum correlation and super quantum correlation. In the following chapter, we define a new quantum game that captures the reduction of uncertainty for the measurement of two non-commuting observables, optimally, with the help of non-local correlation, i.e., entanglement between observed system and quantum memory. Next, we have studied about the protection of information when the information transfers through noisy channel modeled by amplitude damping channel. Finally, in the concluding chapter, we summarize the interesting key results of our work.

Numerical Simulation of Spectral and Timing Properties of Galactic Black Holes

Sudip Kumar Garain

Supervisor: Prof. Sandip Kumar Chakrabarti, Dept. of Astrophysics and Cosmology

A black hole accretion may have both the Keplerian and the sub-Keplerian components. We consider the most general accretion flow configuration, namely, two-component advective flow (TCAF) in which the Keplerian disk is immersed inside a low angular momentum, accreting sub-Keplerian halo component around a black hole. The Keplerian component supplies low energy (soft) photons while the sub-Keplerian component supplies hot electrons which exchange their energy with the soft photons through Comptonization or inverse-Comptonization processes. In the sub-Keplerian component, a shock is generally produced due to the centrifugal force. The post-shock region is known as the CENTrifugal pressure dominated BOUNDary Layer (CENBOL). In this thesis, we study the spectral and timing properties of such accretion flow around non-rotating, galactic black holes using numerical simulations. The radiative properties are studied using a Monte-Carlo code which simulates the energy exchange between the electron and radiation, and the hydrodynamics as well as the thermal properties of the halo are simulated using a finite difference code which uses the principle of total variation diminishing (TVD). These two codes are then coupled and the resulting localized heating and cooling are included in the coupled code. The Keplerian disk is assumed to be the standard Shakura-Sunyaev disk. We simulate several cases by varying the disk and the halo accretion rates. Our results show that the transition from a hard state to a soft state is determined by the mass accretion rates of the disk and the halo. The outflow rate is found to be reduced as a result of enhanced cooling and the emitted spectrum becomes softer. We thus find a direct correlation between the spectral states and the outflow rates of an accreting black hole. We also find that the quasi-periodic

oscillation (QPO) frequency increases and the spectrum becomes softer as we increase the Keplerian disk rate. An earlier prediction that QPOs occur when the infall time scale roughly matches with the cooling time scale, originally obtained using a power-law cooling, is found to remain valid even for Compton cooling. Our findings generally agree with the observations of the black hole candidates.

A Study of Dark Energy from Various Approaches

Nilok Bose

Supervisor: Prof. Archan S Majumdar, Dept. of Astrophysics and Cosmology

It is known from observations that the Universe is currently in accelerated expansion, the cause of which is attributed to a mysterious component called "Dark Energy". There are many innovative ideas in the literature to explain this phenomenon. In this thesis we study the dark energy problem from two different perspectives, viz. (i) scalar field models, and (ii) backreaction from inhomogeneities.

We first show that for a purely kinetic k-essence model the late-time energy density of the universe when expressed simply as a sum of a cosmological constant and a dark matter term leads to a static universe. We then propose our model of k-essence which reproduces the basic features of a standard potential driven inflation in the early Universe and also gives rise to dark matter and dark energy at appropriate subsequent stages. We then present another k-essence model where also we are able to achieve a triple unification. However in this case the inflation is produced through the process of k-inflation. For both k-essence models we show how observational results are used to put constraints on the parameters of this model.

Recently there has been much interest in studying the effect of inhomogeneities on the evolution of the Universe as described by the globally homogeneous FRW metric. In our work we have used the Buchert framework for studying the backreaction from inhomogeneities. Using this framework, in a simple two-scale model, we show that when we include the presence of the cosmic event horizon in our calculations, which inevitably forms when the Universe enters the accelerated phase, backreaction causes acceleration to slow down in the subsequent evolution. Transition to another decelerating era could ensue eventually at a future epoch, ensuring avoidance of a big rip. We also show that the rate of deceleration is more rapid when we consider the event horizon as compared to the case where the event horizon is not considered. We also extend the above model and consider the Universe to be partitioned into multiple overdense and underdense domains, each evolving differently to each other, and study the evolution of acceleration.

Study of the Effects on Lower Ionosphere Due to Solar Phenomena Using Very Low Frequency Radio Wave Propagation

Tamal Basak

Supervisor: Prof. Sandip Kumar Chakrabarti, Dept. of Astrophysics and Cosmology

The ionosphere is a natural detector and it characteristically responds to ionizing actions of solar and other extraterrestrial ionizing agents. Electron and ion chemistry along with the degree of ionization of lower ionosphere evolve with solar radiation intensity. In my research work, I have dealt mainly with the lower ionosphere (60-80 km) i.e., the D-region and the lower E-region using subionospherically propagated Very Low Frequency (VLF) radio signal from a transmitter (Tx) to a receiver (Rx) through Earth Ionosphere Wave Guide. Along with the diurnal changes in the solar flux, the intense hard and soft X-ray spectrum during solar flares greatly perturb the ionospheric D-region and this is sensed by monitoring

the amplitude and phase information of ground based VLF signal. Major part of my thesis is based on the analysis of several physical lower ionospheric parameters using the VLF data of NWC transmitter. The lower ionosphere shows a time dilation in responding to those ionizing agents like solar flares and this property is called the 'sluggishness' of the ionosphere. Through rigorous data analysis, we showed that time delay (Δt) of the ionosphere during the solar flares varies with the strength of the flare ($\phi_{\max}$) and with local solar zenith angle (Z) at flare occurrence time. Moreover, we reported that, correlation between Δt and $\phi_{\max}$ is a strongly Z dependent phenomenon and we stated possible physical explanations for this. Further, using Δt , we developed a new formulation to calculate effective recombination coefficient (α_{eff}) during solar flares using VLF amplitude data ($\Delta A_{\max}$) and simulated D-region electron density ($N_{e,\max}$) using Long Wave Propagation Capability (LWPC) code. Subsequently, we showed that for flares occurred close to local solar zenith, α_{eff} has an inverse relation with $\phi_{\max}$. In another work, we simulated the perturbed environment of lower ionosphere during M and X classes of flares. This consists of using three codes successively, namely, the GEANT4 Monte Carlo simulation, GPI chemical model and LWPC simulation. With reasonable assumptions, this model reproduces the observed VLF signal behaviour during flares. Negative ions are the unique constituent of the D-region and this was estimated using the λ -parameter. We solved electron continuity equation for flare disturbed D-region and using $N_{e,\max}$ from LWPC, we evaluated the variation of λ . Apart from the flare studies, we also studied the quiet global lower ionospheric environment over Indian subcontinent under quiet conditions. Using default simulation model of LWPC, we obtained spatial distribution of VLF signal under ambient solar conditions during sunrise and sunset. Our results agree with observations.

Phase Transition in Black Holes

Dibakar Roychowdhury

Supervisor: Prof. Rabin Banerjee, Dept. of Theoretical Sciences

The present thesis is devoted towards the study of various aspects of the phase transition phenomena occurring in black holes defined in an Anti-de-Sitter (AdS) space. Based on the fundamental principles of thermodynamics and considering a grand canonical framework we examine various aspects of the phase transition phenomena occurring in AdS black holes. We also investigate the critical behavior in charged AdS black holes. The scaling laws for these black holes are found to be compatible with the static scaling hypothesis. Finally, based on the usual framework of AdS/CFT duality, we investigate the phase transition phenomena occurring in charged hairy black holes defined in an asymptotically AdS space. Based on analytic calculations, and using the AdS/CFT dictionary, we explicitly compute the order-parameter for the dual CFT close to the critical point of the phase transition and found that the critical exponent associated with the condensation is $1/2$, which is the universal result of the mean field theory. Moreover, we also find that in the presence of an external magnetic field, the dual CFT exhibit a perfect diamagnetism at low temperatures, which may be regarded as the reminiscent of the so called Meissner effect.

Prepotential Formulation of Lattice Gauge Theories

Indrakshi Raychowdhury

Supervisor: Prof. Manu Mathur, Dept. of Theoretical Sciences

Reformulating gauge theory in terms of gauge invariant loops is an old problem in physics. We reformulate Hamiltonian Lattice Gauge Theory in terms of prepotentials. In prepotential formulation, the gauge invariant or loop operators and states can be analyzed locally. The associated Mandelstam constraints are local and solved exactly to construct

orthonormal loop basis, which is essential if one is interested in the dynamics of the theory in continuum limit (which lies in the weak coupling regime of the lattice theory). We also use prepotential formulation to solve the spectrum of the lattice gauge theory Hamiltonian analytically for a small lattice consisting of four sites.

Dynamics of Neat Ionic Liquid, Binary mixtures and Liquids under Confinement: Theoretical and Simulation study

Snehasis Daschakraborty

Supervisor: Prof. Ranjit Biswas, Dept. of Chemical, Biological and Macromolecular Sciences

In this Thesis, we have presented theoretical studies of Stokes shift dynamics of a fluorescent probe dissolved in pure ionic liquid, and binary mixtures of it with various common dipolar solvents. In addition, theoretical study on how charge-charge interaction decouples from orientational relaxation in ionic liquids, and computer simulations on structural and dynamical features of various model liquids are also presented. Ionic liquid, being an environmentally benign solvent, has been attracted interests by many researchers molecular level investigation. Moreover, it has been shown that ionic liquids possess micro-heterogeneity with strong implications on various relaxation processes. This thesis therefore primarily focuses on understanding relaxation dynamics in terms of microscopic picture. We have developed molecular theories for this purpose and molecular mechanism has been ascribed via facilitating direct comparison between theoretical predictions and measurements. In some cases, where experimental data are not available yet, our predictions on dynamical features motivate new experiments and/or simulations. Recent fluorescence upconversion measurements of (ionic liquid + water) system have revealed semi-quantitative agreement between experimental data and our theory. We have also developed a molecular theory for understanding the dielectric relaxation of ionic liquid where we have focussed on the importance of dipole-dipole, ion-dipole and ion-ion interactions for their relative roles in dielectric relaxation and collective rotation. Computer simulations have been carried out to understand the structural and dynamical behaviours of model liquids.

The thesis contains eleven chapters including Introduction (Chapter 1), describing the motivations of the works presented in the thesis with literature survey, and Conclusion (Chapter 11), where main results in various works are summed-up and some future problems discussed. In Chapter 2 and 3 we have discussed our theoretical understanding on the Stokes shift dynamics of two non-conventional ionic liquids. Chapter 4 consists of the theoretical study of solute probe dependence on Stokes shift dynamics in ionic liquid. The probable origin of ultrafast time scale, originated from Three Pulse Photon Echo Peak Shift (3PEPS) measurements for ionic liquid has been described in Chapter 5. Chapter 6 and 7 deals with the theoretical study of Stokes shift dynamics of a solute probe in binary mixture of ionic liquid and dipolar solvent. We have described in Chapter 8 the theoretical description for the study of dielectric relaxation in ionic liquid. Chapter 9 and 10 describes the computer simulation investigation of dynamics of some model liquids.

Mean Field Theory and Computer Simulations on Non-Equilibrium Phenomena in Complex Chemical Systems

Amit Das

Supervisor: Dr. Jaydeb Chakrabarti, Dept. of Chemical, Biological and Macromolecular Sciences

Studies of non-equilibrium phenomena form the core of physical chemistry research on complex chemical systems. In the present thesis, we investigate a host of important non-equilibrium phenomena in various

complex chemical systems. We explore different aspects of dipolar solute rotation in various complex solvent media, like the supercritical fluids¹, common dipolar liquids², ionic liquids³ and electrolyte solutions³, to develop a generalized molecular theory of solute rotation. We incorporate the effects of both solvent structure through molecular hydrodynamic solvent static structure factor, and solute-solvent electrostatic interactions, within mean-field framework. Our approach satisfactorily describes¹⁻³ the experimental rotation times and provides microscopic explanation for the overwhelming domination of hydrodynamic contributions over the electrostatic contributions^{2,3}, apparently indicating quasi-universality³.

Next, we have studied the dimensional crossover⁴, observed in fluids under nanoscale confinements, using computer simulations. We provide a generic understanding of the crossover as a manifestation of confinement-induced modifications in long-wavelength behaviour of both equilibrium and dynamic density fluctuations⁴. Exploring the effects of confinement and different confining potentials on non-equilibrium solvation dynamics, we bring out qualitatively different mechanisms⁵ of slowing down of solvation dynamics in solvophilic and solvophobic confinements. If the surrounding bulk solvent is subcritical near the liquid-gas coexistence, we show⁶ that a competition between wetting by solvophilic solute and drying by solvophobic walls produce dramatic effects.

We have studied various aspects of conformational fluctuations in biomacromolecules using all atom molecular dynamics simulations. The thermodynamics of conformational changes in biomacromolecular complexes is extracted from a histogram-based method⁷ using dihedral angles as conformational variables. Our conformational thermodynamics data for protein-peptide complexes⁷ corroborate well with the experimentally observed conformational and binding entropies, while the data for metal-ion binding to a protein⁸ correlate well with the experimental observations. From dynamic conformational fluctuations we explain⁹ non-equilibrium allosteric regulation in a protein in terms of changes in pattern of dynamic correlations among dihedral angles upon metal-ion binding. We quantitatively characterize the thermodynamics of interfacial changes in a protein-protein complex¹⁰, including the conformational and water contributions, and changes in interfacial water dynamics.

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7. A. Das, J. Chakrabarti and M. Ghosh, Conformational contribution to thermodynamics of binding in protein-peptide complexes through microscopic simulation, *Biophys. J.* **104**, 1274 (2013).

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9. A. Das, M. Ghosh and J. Chakrabarti, Dynamic correlations among allosterically regulated conformational variables in biomacromolecules, *Communicated* (2013).
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Studies on Biomolecular Recognition Using Ultrafast Laser Spectroscopic Techniques

Tanumoy Mondal

Supervisor: Prof. Samir Kumar Pal, Department of Chemical, Biological & Macromolecular Sciences

“Biomolecular recognition” process refers to the weak non-covalent interaction which takes place selectively and specifically between small ligand/drug molecules with biological macromolecules. Understanding of molecular recognition in biological (like DNA, proteins) and bio-mimetic (like micelles, reverse micelles, vesicles etc.) environment is the central attraction for drug designing and for the discovery of new medicine to benefit human health. In this respect, time-resolved fluorescence spectroscopy is an efficient tool to study the process of biomolecular recognition. In the proposed presentation, the interaction of biologically relevant drug molecule (Rifampicin) with model drug delivery system like micelle (Sodium dodecyl sulfate, SDS and Cetyl trimethyl ammonium bromide, CTAB) will be discussed. The interaction of rifampicin with a model drug carrier protein in human blood plasma (Human Serum Albumin, HSA) will also be discussed in this course of presentation. The binding pocket of the drug, and its competitive interaction with other drug (Warfarin) in a physiologically relevant environment will be highlighted. In the next part of my presentation, I will be discussing about some specific protein-DNA and protein-protein interactions which are crucial mechanisms in signaling cascades leading to cellular events like regulation of gene expression and transcription. In this section, the use of numerous spectroscopic techniques to understand the recognition of specific operator DNA sequences by lambda repressor protein, and repressor-repressor interaction, which regulates the lysogenic cycle of bacteriophage lambda, will be talked about. Moreover, the detailed chemical principles of the conformation-dependent electron transfer reaction from protein to DNA, governed by differential protein dynamics upon binding to different DNA target sequences will also be discussed.

Spectroscopic Studies on Photoreactivity of Inorganic Nanocrystals and Medicinally Important Organic Dyes

Soumik Sarkar

Supervisor: Prof. Samir Kumar Pal, Department of Chemical, Biological & Macromolecular Sciences

‘Photoreactivity’ is a general name for a group of rather different types of reactions occurring in most redox-active systems, including inorganic nanostructures associated with some organic dyes having some medicinal significance. It is well-recognized that optical radiation can change the properties in those inorganic-organic nanohybrid materials and the great majority of those materials absorb UV and an appreciable amount of visible radiation. Therefore, absorption is a first indication that a compound may participate in a photochemical process, thereby having the potential of being photoreactive. The importance of photoreactivity of some organic dyes lies in various fields of science like photodynamic

therapy, bioremediation in biomedical applications. Some of the medicinally important organic dyes are also well-known as photosensitizers. All of these photoreactivities of a photosensitizer are associated with ultrafast electron or electronic energy transfer processes from a donor to an acceptor molecule, but the degree and character of excited-state deactivation varies strongly from case to case. Therefore, ultrafast spectroscopic technique is an ideal tool for probing such charge carrier dynamics in nanohybrid materials. The key focus of this thesis is to investigate the excited-state dynamics of nanomaterials when they are in a close proximity of other organic, inorganic and biological macromolecules, which is important from both fundamental and application perspectives, such as, light-harvesting devices, efficient photocatalysts and phototherapeutic agents. For example, we have explored a novel mechanism for ZnO NP-sensitized BR degradation *via* defect-mediated nonradiative energy transfer pathway, and rigorous medical trials are likely to offer better phototherapeutic improvements in the treatment of hyperbilirubinemia. By using a picosecond-resolved Förster resonance energy transfer (FRET) technique, we have demonstrated the role of the gold layer in promoting photoinduced charge transfer from ZnO-Au nanocomposite to a model water contaminant. Due to the formation of the Schottky barrier at the ZnO-Au interface and the higher optical absorptions of the ZnO-Au photoelectrodes arising from the surface plasmon absorption of the Au NPs, enhanced power-conversion efficiency was achieved compared to bare ZnO-based dye-sensitized solar cells (DSSCs). In another study, potential cosensitization of extrinsic sensitizer CdTe QDs in ZnO nanorod-based DSSCs has been established, and the multipath enhancement offered in this device architecture results in an increased and extended photoresponse with respect to the individual materials employed. We have also revealed that biomolecules and NPs can be linked to prepare a novel multifunctional bio-nanocomposite that is able to recognize and efficiently reduce target organic molecules. Another study provides a mechanistic explanation for the ultrafast excited-state deactivation by considering every single aspect of the quenching mechanisms, namely photoinduced electron transfer (PET), FRET and nanosurface energy transfer (NSET) from the host porous alumina membrane to different guest molecules, which may find its importance in the use of porous alumina in light-harvesting devices. Finally, we have demonstrated the exciting potential of porphyrins as light-harvesting green dyes that can simultaneously be used in visible-light photocatalysis (VLP) and photovoltaics.

List of Publications

1. **S. Sarkar**, A. Makhal, T. Bora, K. Lakshman, A. Singha, J. Dutta and S. K. Pal "Hematoporphyrin-ZnO Nanohybrids: Twin Applications in Efficient Visible-Light Photocatalysis and Dye-Sensitized Solar Cells", *ACS Appl. Mater. Interfaces*, 4 (2012) 7027-7035.
2. **S. Sarkar**, A. Makhal, K. Lakshman, T. Bora, J. Dutta and S. K. Pal "Dual-Sensitization" via Electron and Energy Harvesting in CdTe Quantum Dots Decorated ZnO Nanorod-Based Dye-Sensitized Solar Cells, *J. Phys. Chem. C*, 116 (2012) 14248-14256
3. **S. Sarkar**, A. Makhal, S. Baruah, M. Mahmood, J. Dutta and S. K. Pal "Nanoparticle-Sensitized Photodegradation of Bilirubin and Potential Therapeutic Application", *J. Phys. Chem. C* 116 (2012) 9608-9615 (Nature-India Highlighted).
4. **S. Sarkar**[‡], A. Makhal[‡] and S. K. Pal ([‡]contributed equally) "Protein-Mediated Synthesis of Nanosized Mn-doped ZnS: A Multifunctional, UV-Durable Bio-Nanocomposite", *Inorg. Chem.* 51 (2012) 10203-10210.
5. **S. Sarkar**[‡], A. Makhal[‡], H. Yan, D. Wulferding, F. Cetin, P. Lemmens

and S. K. Pal ([‡]contributed equally) Ultrafast Excited State Deactivation of Doped Porous Anodic Alumina Membranes, *Nanotechnology*, 23 (2012) 305705

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First Principle study of Novel Materials

Sudipta Kanungo

Supervisor: Prof. Tanusri Saha-Dasgupta, Dept. of Condensed Matter Physics & Material Sciences

This thesis is devoted to the study of microscopic origin of many exciting and intriguing physical properties of different complex and novel materials, employing primarily first principles technique. In particular, we have studied three different category of compounds, namely i) perovskite structured transition metal oxides, (Sr,Ca)RuO₃ and BiCoO₃, ii) low dimensional quantum spin systems Sr₃BB'O₆ (B=Ni/Cu, B'=Pt/Ir) and Zn₂VO(PO₄)₂ in pristine and Ti doped form, and iii) metalorganic compounds, Mn-succinate and Fe-Nb coordination polymer. The major findings of our study may be summarized as,

(1) We explain the contrasting magnetic behavior of two isovalent perovskites SrRuO₃ and CaRuO₃, in terms of active role of nonmagnetic cationic 'A' site [1,2], which is supported by experimental measurements. We settle down the controversy of spin states of Co and crystal symmetry of BiCoO₃ [3] in both ambient pressure and high pressure phase which is found to be guided by the covalent mixing between O-*p* states with Bi lone pair *s* and *p* states.

(2) We figure out the low energy spin models of low dimensional quantum spin systems Sr₃NiPtO₆, Sr₃CuPtO₆, Sr₃NiIrO₆ [4] in terms

of ab-initio calculation of magnetic exchanges as well as anisotropy energies. From microscopic analysis we confirm that $\text{Zn}_2\text{VO}(\text{PO}_4)_2$ should be considered as a 2D square lattice spin 1/2 system instead of previous prediction of 1D spin 1/2 system. We also predict a new magnetic ground state of $\text{Zn}_2\text{VO}(\text{PO}_4)_2$ by chemical substitution of Ti in place of V, which can be verified in terms of future experiment [5].

(3) Using the knowledge of exchange interactions we explain the unusual two step magnetic ordering of the Mn spins in organic-inorganic hybrid system $\text{Mn}(\text{C}_4\text{H}_4\text{O}_4)$ which is rare in conventional inorganic system [6]. We predict novel spin state transitions and external stimuli driven change in magnetic ordering in metalorganic Fe-Nb coordination polymer [7].

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Magnetic and Optical Studies of Wide Band-Gap Oxide Semiconductors

Shyamsundar Ghosh

Supervisor: Prof. Kalyan Mandal, Dept. of Condensed Matter Physics & Material Sciences

The exploitation of electron spin and charge degree of freedom in a single host semiconducting materials, named dilute magnetic semiconductors (DMSs) have drawn huge research attention for development of new spin-based electronics, called spintronics [1]. Stabilization of carrier spin polarization (ferromagnetic ordering) in wide-band ($E_g \geq 3.0$ eV at 300K) oxide semiconducting hosts such as SnO_2 , ZnO , HfO_2 , TiO_2 etc. has special advantages due to their unique optical properties [2]. In this thesis, we have investigated the role of different transitional metal (TM) or rare-earth (RE) impurities and vacancy-type defects such as cation (Zn, Sn) or anion (O) vacancy in stabilizing room-temperature (RT) ferromagnetism (FM) in wide-band oxide semiconductors with the correlation of their optical as well as electrical properties. We found absence of intrinsic FM in TM Co-doped ZnO and SnO_2 bulk powders prepared by mechanical milling process. Although the divalent Co ions are substituted at Zn or Sn site within ZnO or SnO_2 lattice, no evidence of intrinsic FM is detected, instead a paramagnetic behavior is observed [3, 4]. However, with the reduction of particle size to nanoscale regime (< 50 nm), room-temperature ferromagnetism (RTFM) is found to be stabilize in Co-doped SnO_2 which decreases or even vanishes when the samples are annealed in oxygen atmosphere. This indicates that FM associated with the nanostructures arises due to structural defects, not due to the substituted Co ions [4]. In Fe-doped SnO_2 bulk materials, an evidence of antiferromagnetic (AFM) interaction between the Fe^{2+} ions are confirmed though Zero

field-cooled (ZFC) and field-cooled (FC) magnetization studies whereas with the incorporation of additional nitrogen (N) at O site, ferromagnetic interaction between Fe^{2+} ions mediate through the holes arising due to N co-doping [5]. Therefore, sufficient carrier concentration might be essential criteria to turn on the FM interaction between the TM ions substituted within the host lattice. Similar to pure SnO_2 nanorods, pure SnO_2 thin films prepared by radio-frequency (RF) magnetron sputtering technique also exhibited RTFM which interestingly, decreased gradually with RE ion Gd-doping [6]. Photoluminescence (PL) and electron paramagnetic resonance (EPR) spectroscopic analysis showed that structural defects such as oxygen vacancy (V_O) are the dominant source for the origin of magnetic moment in pure SnO_2 nanostructures [7]. Defect-driven d^0 RTFM are also observed in case of pure ZnO nanowires (NWs) fabricated within the nanopores of anodic aluminium oxides (AAO) template. This FM signature in ZnO NWs has enhanced significantly with doping of non-magnetic group-1 element potassium (K) up to a certain concentration limit. PL spectroscopy showed the evidence of large concentration of Zn vacancy (V_{Zn}) which stabilized due K-substitution at Zn site [8]. K-doping also introduces a hole at O site which mediate the FM interaction between the V_{Zn} defects. Substitution of Lithium (Li) at Zn site also found to stabilize high T_C FM in ZnO NWs. It is observed that saturation moment as well as the Curie temperature in Li-N co-doped ZnO NWs can be enhanced by increasing N concentration [9]. This indicates the role of holes to mediate FM interaction between the Zn vacancies in $\text{ZnO}:\text{Li}$ matrix. On the other hand, F co-doping which donates electron into the system acts to oppose the FM interaction in Li-F codoped ZnO [9]. A comparative study regarding the degree of efficiency of different alkali metals like Li, Na, K etc. to induce FM in ZnO thin films, prepared by pulsed laser deposition (PLD) is also performed and it is found that Li is the most effective alkali element compared its other co-group candidates. Effects of oxygen partial pressure (PO_2) and film thickness on the magnetic, optical and electrical properties in sodium (Na)- ZnO thin films are also investigated [10]. At last, positron annihilation spectroscopy (PAS) is employed to investigate the presence of different defects and their evolution depending on annealing temperature and atmosphere TiO_2 and also due to Li-substitution in ZnO nanoparticles [11]. It is found that Li-substitution indeed enhances the V_{Zn} defect concentration which is responsible to stabilize d^0 FM in Li-doped ZnO . Therefore, our study shows that substitution of nonmagnetic group-1 alkali-metal in ZnO can be a promising direction to stabilize, enhance and tune high T_C FM and this can be an exciting approach to prepare new class of ZnO based DMS for spintronic and opto-spintronic applications.

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Synthesis of transition metal based magnetic nanostructures and their characterization for suitable applications

Debasish Sarkar

Supervisors: Prof. Kalyan Mandal and Dr. Madhuri Mandal, Dept. of Condensed Matter Physics and Material Sciences

Study of nanostructured magnetic materials become an area of immense research interest as they provide the fundamental building block for nanoscience and nanotechnology. Due to their extremely small dimension as comparable to some characteristic length scales of materials such as Bohr exciton radius, spin diffusion length, carrier mean free path, magnetic domain wall width etc., they often exhibit some novel and enhanced properties over their bulk counterpart [1-3]. These novel properties can also be tailored through their controlled organization in the form of various interesting nanostructures [2]. In this thesis we have investigated different morphology dependent properties of transition metal and metal oxides (especially iron and its oxides). We have also analyzed the effect of some other metallic, metallic oxide or semiconducting materials on the intrinsic properties of these transition metals and their oxides. We have prepared different nanostructures of iron (Fe), Nickel (Ni), α -Fe₂O₃ and Fe₃O₄ through both template assisted and non-template routes.

Magnetite hollow spheres of different sizes have been prepared through a template free solvothermal technique [4]. Hollow nature of these spheres is very useful for encapsulation of proteins, different drugs, dyes etc., their magnetically guided transport and finally their controlled release at targeted tissues. Magnetic domain changes from pseudo single domain (PSD) to multi domain (MD) configuration with the increase of size and shell thickness of these spheres. High surface area and hollow interior of these spheres also improves their adsorption capability which makes them useful in adsorption of dyes (Eosin, Methylene blue), heavy metals (As) etc. from ground water [5]. Nanochains of Fe, Ni, α -Fe₂O₃ and Fe₃O₄ have been prepared by using DNA as template material [6, 7]. DNA being a chainlike molecule directs the growth of the nanoparticles in chainlike fashion. The surface of Fe and Ni nanoparticles has modified by thin layer of Au which makes them very stable without affecting their magnetic properties significantly. However, the DNA template is found to affect significantly on the magnetic properties of these materials. We have also prepared nanowires (NWs) of α -Fe₂O₃ with high aspect ratio and improved their magnetic, photoluminescence, electrically conductive properties through their surface modification by some magnetic and non-magnetic materials [8, 9]. We have investigated the electrochemical properties of these NWs and also improved it by several orders of magnitude via modification of the NW surface with MnO₂. These NWs have high energy as well as high power density at higher scan rates which is very important for their use as supercapacitor electrodes and also as electrode material in Li-ion batteries.

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Chern Simons theory in the context of 2+1 and 3+1 quantum gravity

Rudranil Basu

Supervisor: Prof. Samir Kumar Paul & Dr. Parthasarathi Majumdar, Dept. of Condensed Matter Physics and Material Sciences

During the course of my PhD, I have worked on some particular aspects of Chern Simons theory, which are relevant in studies on quantum gravity. In 3 space-time dimensions these studies focus mainly on spin-2 pure gravity, without propagating degrees of freedom. Being devoid of local degrees of freedom, this gauge theory is classically trivial, with a finite number of global degrees of freedom (in absence of boundary). We introduced a new coupling parameter in the theory in order to make it consistent at the quantum level. Moreover we went on to find a particular discrete set of allowed values of this coupling. In the context of 4 dimensions, we were successful in resolving a confusion regarding quantum (logarithmic in horizon area) correction to black hole entropy. The afore-said confusion did arise regarding the gauge group of the Chern Simons theory. Chern Simons here works as an effective field theory which dictates dynamics of horizon (black horizons are special cases). Two approaches, starting with an SU(2) and a U(1) group apparently gave different results. We showed how and why both the approaches should give an unanimous result.

Quasistatic and Ultrafast Magnetization Dynamics in Magnetic Nanostructures

Bivas Rana

Supervisor: Prof. Anjan Barman, Dept. of Condensed Matter Physics and Material Sciences

Nanomagnets are interesting systems for future applications in nanotechnology including in patterned magnetic media, magnetic data storage, magnonic crystals, magnetic logic, sensors, and biomedical applications. All applications require the knowledge base of the magnetization processes of nanomagnets and their arrays at various time and length scales. In this thesis, we have studied the quasistatic and ultrafast magnetization dynamics of lithographically patterned magnetic nanodot arrays and chemically synthesized clusters and chains of magnetic nanoparticles. The quasistatic magnetization reversal dynamics is studied by static magneto-optical Kerr effect (SMOKE) microscope and vibrating sample magnetometer (VSM), whereas the ultrafast magnetization dynamics is studied by a home-built all-optical magneto-optical Kerr effect (TRMOKE) microscope with collinear pump-probe geometry. The experimental results are explained with the aid of numerical micromagnetic simulations. We have investigated the magnetization dynamics of two-dimensional arrays of Ni₈₀Fe₂₀ (permalloy) nanodots of two different shapes (square and circular), with varying sizes between 200 nm and 50 nm, and with varying inter-element separations of the arrays between 50 nm and 400 nm. A transition from strongly collective dynamics to completely isolated dynamics through various weakly collective regimes (in picosecond magnetization dynamics and quasistatic reversal dynamics), variation of precession frequency and damping with the interdot separation, transition from strongly collective dynamics to non-uniform collective dynamics and damping with applied bias field magnitude, effects of dipolar and quadrupolar interdot interactions, effects of the variation of dot size on the dynamics of

single elements and arrays, and anisotropy of collective dynamics have been thoroughly studied by experimental and micromagnetic simulation results. A significant variation of the magnetization relaxation times are observed with dot size, shape and area density of array, whereas the femtosecond demagnetization times remain unchanged. The magnetization reversals of chains and clusters of exchange-coupled magnetic nanoparticles occur through the formation of various local domain states including vortices, fanning- and curling-like modes, depending upon the cluster geometry, whereas constituent nanoparticles reverse by the quasi-coherent rotation of magnetization. In ultrafast magnetization dynamics, the relaxation times and precessional modes frequencies vary significantly with the clustering geometry, whereas the demagnetization times remain unchanged.

Magnetism in dilute magnetic semiconductors and oxides

Hirak Kumar Chandra

Supervisor: Prof. Priya Mahadevan, Dept. of Condensed Matter Physics and Material Sciences

In this thesis I have studied the electronic structure and magnetism in dilute magnetic semiconductors as well as oxides using examples which range from defects in semiconductors, the most well studied example of a dilute magnetic semiconductor- Mn doped GaAs, δ -doped heterostructures of GaAs/Mn, transition metal doping in the well known ferroelectric oxide BaTiO_3 as well as B doping/diffusion into the insulating tunnel barrier region in MgO .

The field of spintronics began with the doping of conventional semiconductors with transition metal atoms, thereby rendering them magnetic. The choice of conventional semiconductors for this purpose was the hope that one could investigate this new technology with the existing semiconductor technology. However the doped materials had properties entirely different from the undoped ones. Further, one found that several examples exhibited magnetism even in the absence of doping. With the discovery of magnetism in HfO_2 which has no magnetic element in it, the field of magnetism in intrinsic oxide semiconductors has received a lot of interest. It was realized that the same material prepared by different synthesis routes may or may not show magnetism. It has been seen later that, the dependence of magnetism on different synthesis routes was due to the defects introduced into the systems during growth. These defects play a crucial role to drive the system magnetic. We have taken ZnO , a compound semiconductor, for our analysis. This system has been extensively studied in the literature. We have examined the local moment formation for different possible types of defects in ZnO such as Zn-vacancy, O-vacancy, Zn-interstitial, O-interstitial etc. For our calculations we have used ab-initio spin polarized density functional theory. A supercell of ZnO is constructed and the defects mentioned above are introduced into that supercell. We then go on to examine if the moment formation in these systems can be described as arising due to the Stoner mechanism. Few basic rules emerge from the analysis which can help us predict which defects would show an induced magnetic moment and which ones will not.

The field of dilute magnetic semiconductors is plagued by the issue of defects, inhomogeneous doping, multiple phases etc. which complicate the experimental results on these systems and one is not sure which results are intrinsic to the system. Mn doped GaAs is a system which has been extensively studied and the magnetism there is believed to be intrinsic. However the basic electronic structure of Mn doped GaAs has been repeatedly questioned, especially in recent times. The issue whether

Mn doped GaAs corresponded to a valence band hole scenario or impurity band hole is central to our understanding of magnetism. In order to examine this aspect, we have studied the electronic structure of Mn doped GaAs in model multiband Hubbard calculations. The impurity band picture is obtained within our calculations. In addition as Mn doped GaAs belongs to the charge transfer metal (p-d) limit, Coulomb interactions on Mn do not drive the system insulating. Quantum confinement effects we go on to show can drive the system into the Mott-Hubbard regime and hence drive the system insulating for small values of U .

DMS systems are limited in their applications because of their low ferromagnetic Curie temperature (T_c). A lot of experimental efforts have been devoted to make materials which can exhibit room temperature ferromagnetism. It has been reported that ferromagnetic T_c and spontaneous magnetization of DMS materials depends on the distribution of impurities. Based on this idea T_c can be enhanced significantly in some low dimensional DMS systems. A possible way to achieve this is to synthesize materials in which a two dimensional layer with doped magnetic atoms has been sandwiched within bulk semiconductors. A δ -doped magnetic heterostructure is nothing but highly doped thin magnetic semiconductor layers followed by thick nonmagnetic semiconductor layers. These types of heterostructure systems are of interest because a large number of magnetic ions can be doped in a thin layer which cannot be realized in bulk Mn doped GaAs system. Here, we have theoretically investigated with the help of first principle density functional calculations, what are the magnetic interactions one finds when Mn is doped into a layer of GaAs heterostructures. This analysis has been carried out at various doping concentrations.

The tunnel magnetoresistance (TMR) property of some insulating materials has attracted a lot of research interest as the materials possessing this particular property have potential applications in magnetic random access memory and magnetic read heads. TMR is a magnetoresistive effect that occurs in magnetic tunnel junctions (MTJs). The MTJs consist of two ferromagnetic materials separated by a thin insulating layer. The insulating layer is made thin enough so that the electrons can tunnel from one ferromagnetic material to the other. This process is forbidden classically, so TMR is purely a quantum phenomena. We have studied the role of B in the CoFeB/MgO/CoFeB type of tunnel junction. According to recent experimental reports, the B atom diffuses into the MgO layer during annealing. B that diffuses into the MgO layer during annealing could modify the TMR for the thin oxide tunnel junction. We have investigated certain sites B can occupy in MgO , (i) B on Mg, (ii) B on O and (iii) interstitial B. We have observed that when B goes to different sites in the MgO crystal, it could introduce spin polarized defect states into the system. We have compared the formation energies for these three possible types of configurations using ab-initio density functional theory. The configurations that are favored are the nonmagnetic ones. These defects introduce mid-gap states inside the band-gap of MgO , reduce the effective band gap of the material and hence we predict that they could also affect the TMR ratio.

Multiferroic materials are those in which one finds the coexistence of magnetism and ferroelectricity. The study of these materials has become an active area of research during the last one or two decades. There are very few naturally occurring materials which can simultaneously exhibit magnetism and ferroelectricity among the perovskite oxides. A well known example of a ferroelectric material is BaTiO_3 . Here the Ti remains in Ti^{4+} oxidation state which has $3d^0$ electronic configuration. The large ferroelectric polarizations found in the d^0 compounds is associated with the large offcentric distortions, that one finds in these systems.

Ferroelectricity is also seen in compounds with a finite d electron count, however the polarization values are small in these cases. Therefore if we can construct some compounds which have d^0 type distortions with finite d electron count, that would be a possible route to multiferroic materials. In order to examine this we have studied the stabilization of d^0 type distortions as electrons are doped into BaTiO_3 compound. This has been achieved by doping transition metal atoms as we could then have both magnetism and ferroelectricity. We have performed ab-initio density functional calculations using the GGA +U form for the exchange-correlation functional. The ferroelectric stabilization energies have been calculated for different types of doping. Several instances where ferroelectric distortions survive have been found. These ideas of the dilute doping limit are used to predict bulk multiferroics.

EVLP REPORT

The following Bose Colloquia and The Institute Colloquia/Seminars were held:

BOSE COLLOQUIUM

1. *Speaker:* Dr. Suresh Das

Affiliation: Director, Photosciences and Photonics Section, Chemical Sciences and Technology Division, National Institute for Interdisciplinary Science and Technology, (CSIR), Trivandrum

Title of the Colloquium: Photoresponsive Materials

Date: 03.05.2013

2. *Speaker:* Dr. R. Chidambaram

Affiliation: Principal Scientific Adviser to the Govt. of India & Chairman, Scientific Advisory Committee to the Cabinet (Former Chairman, Atomic Energy Commission)

Title of the Colloquium: The Research & Innovation Ecosystem

Date: 28.06.2013

INSTITUTE COLLOQUIUM / SEMINAR

1. *Speaker:* Dr. Jak Chakhalian

Affiliation: Charles and Claudine Scharlau Professor of Physics Director, Laboratory for Artificial Quantum Matter Physics Department, University of Arkansas, USA

Title of the Seminar: That strange copper oxide

Date: 22.05.2013

2. *Speaker:* Dr. John W. Freeland

Affiliation: Physicist, Advanced Photon Source, Argonne National Laboratory, Argonne

Title of the Seminar: Understanding Interfaces as a Route to Control the Orbital Degree of Freedom in Cuprates

Date: 27.05.2013

3. *Speaker:* Dr. G. Narahari Sastry

Affiliation: Centre for Molecular Modeling, Indian Institute of Chemical Technology, Hyderabad, India

Title of the Seminar: Modulating Non-Bonded Interactions: The Causes and Consequences

Date: 17.06.2013

4. *Speaker:* Prof. Tapas Chakraborty,

Affiliation: Sr. Professor and Head, Dept. of Physical Chemistry, Indian Association for the Cultivation of Science, Jadavpur, Kolkata

Title of the Seminar: Methyl rotor in chemistry and spectroscopy

Date: 05.07.2013

5. *Speaker:* Dr. Jahur Alam Mondal

Affiliation: Scientific Officer (E), Radiation & Photochemistry Division, Bhabha Atomic Research Centre, Mumbai

Title of the Seminar: Structure and Orientation of Water at Model Membrane Interfaces: A Heterodyne-Detected Vibrational Sum Frequency Generation Study

Date: 26.07.2013

6. *Speaker:* Dr. Nilmoni Sarkar

Affiliation: Professor, Dept. of Chemistry, IIT-Kharagpur, W.B.

Title of the Seminar: Chemistry in Microheterogeneous Media: Investigation of Various Photophysical and Dynamical Phenomena

Date: 30.08.2013

SUMMER RESEARCH PROGRAMME, MAY-JULY 2013

The Summer Research Programme is designed for students in first/second year of M.Sc in Physical, Chemical (including Biophysics and Chemical Biology) and Mathematical Sciences for a period of eight weeks (with no break) under the supervision of a Faculty Member of SNBNCBS in an area of mutual interest.

- 22 students enrolled for the 8 weeks in-house programme.
- 10 funded students (Fellowships from KVPY, INSPIRE & Indian Academy of Science). The rest were funded by SNBNCBS.
- On completion of 8 weeks, students deliver an Open Talk and submit 3 copies of their project work for the Library, EVLP office and their respective Supervisor.
- Certificate & stipend are given to students on completion of the programme.

EVENTS

Independence Day Celebration



Avijit Ganguly

Come August 15 and all minds buzz with the reminiscence of the moment when India was freed from foreign rule and a nation was born in 1947. S. N. Bose National Centre for Basic Sciences solemnly observed the 67th Independence Day. A bright sunny morning, the green lawn decorated with miniature tricolours, music-system airing patriotic numbers and academicians and staff members assembled under the main porch – all set to a mood of celebration. Prof. A. K. Raychaudhury, Director, took the salute at the Security Guards' march-past and hoisted the Indian National Flag while the National Anthem was being sung by all present in the ceremony. The Director paid homage to S. N. Bose, the scientist whom the centre is named after, by garlanding his bust. A hearty gathering of faculty members, students and staff for tea followed.

STUDENTS' PAGE

“Geetosudharoshe Esho”: Centenary celebrations of Tagore receiving Nobel Prize in Literature*Hrishit Banerjee*

On 2nd of August The Centre organised a programme to commemorate the 100th year of Rabindranath Tagore receiving the Nobel Prize in literature for his work “Song Offerings” popularly known as “Geetanjali” in Bengali. The programme started with our Director, Prof. Arup Kumar Raychaudhuri lighting the ceremonial lamp to mark the beginning of the programme which was subsequently followed by his address. Up next was an illuminating talk by Prof. Sukanta Chaudhuri, an eminent Emeritus Professor of the esteemed Department of English of Jadavpur University on the recently developed website “Bichitra”: The Online Tagore Variorum, a project of the School of Cultural Texts and Records of Jadavpur University, in association with Rabindra Bhavana, Visva-Bharati.

A cultural programme “Geetosudharoshe Esho” was also a part of the event organised by the students of the Centre. Starting with an inaugural dance by Anuradha Das paying homage to Tagore, by showering flowers on his image, followed by eloquent performances of recitation by Ambalika Biswas and Ruma Mandal, respectively, which incidentally depicted Tagore's wish to be read and performed over and over again through centuries to come.

Another dance recital by Anuradha Das followed which aptly captured the mood of the verse depicting the philosophical essence of the verses of “Geetanjali”, the shower of love and blessings from The Supreme Being.

This particular philosophical train of thought formed the cornerstone of the songs in “Geetanjali” and the next and last part of the programme “Prabhu Amar Priyo Amar” was thus a musical elocution, a scripted performance of vocal renditions of Tagore songs from “Geetanjali” and narratives of English transcreations of some of his verses, with vocal performance by Pratik Tarafdar, Tamisra Pal, Anirban Karmakar, Ishita Duttachoudhury, narratives by Ambalika Biswas and Ruma Mandal, script, narration and vocals by Hrishit Banerjee and percussion accompaniment by Debasish Dasmahanta respectively, conveying this duality of thought, of seeing the Lord in one's love and vice versa which was very evident in most of Tagore's works, and which held the western world in awe of his musings.

The programme concluded with our Director, Prof. Raychaudhuri's generous offer of assistance to the students to set up the S.N.Bose Centre Recreation Club to promote cultural and recreational activities at the Centre.

SNB Football Diaries: 2013*Biplab Bhattacharjee*

For the football lovers of SNB, here are a few pages of my diary describing, through my eyes, the Football League-2013 of SNB, in compact form to meet the space constraints of the newsletter.

11th August 2013

The football passion went viral today at SNB with another session of SNB Football League scheduled to be played from tomorrow. Today we, all the football lovers of SNB gathered at the ground to select the

final team line up of the teams and to decide the format of the tournament. After a lot of ifs and buts the line up of three teams, The Royal Tigers, The Royal Hunters and The Royal Rangers have been finalized. Each team will play two games in the league stage, facing the other two teams. Best two teams will be playing the final.

12th August 2013

The tournament kicked off today. It was though another day for the footballers playing against each other on a daily basis, but with cheerful spectators around and some enlightened tournament spirit, it is always a nervous affair. We, The Royal Hunters turned out to be better in controlling the nerves and beat The Royal Rangers 4-1 in the first encounter. Scoring four goals in the first match, we seem to have found the right combination going for the rest of the tournament.

13th August 2013

With a winning boost we took the field today, confidently, to play against the Royal Tigers. This match seemed to be a better competed one with the strikers of Royal Tigers, Soumyakanti, Ransell and Sabyasachi, showing their skills gleefully. However, with a strong defense offered by Ashutosh, Debasish and Arindam and few good attacks centred around Manotosh da, Tilak da and myself, it was a hard fought win for us, with the scoreline reading 4-3. With two wins in a row we are all set for the final.

14th August 2013

The last match of the league between the Rangers and the Tigers, today, was a semi-final for both the teams as a win could take the winning team through to the final. However, with more scored goals Tigers could have fancied their chances even with a draw. The game started with both the teams looking defensive. However, the opposition soon went ahead with two goals. Sabyasachi scored the lone goal for the Tigers which was not sufficient and amidst a lot of heated arguments on and off the field, Tushar Nandi took his team to the final with a couple of goals to his name.

15th August 2013

The final, scheduled to be played today, was washed out due to heavy rains. It has been a gloomy day for the happy finalists and the enthusiastic spectators as well. It seems to continue for some more days and the match will be played when nature permits.

24th August 2013

At last we played the final of the tournament today in a very short notice, and both the teams (Royal Hunters and Royal Rangers) took the field almost unprepared to lock horns. As the beginning shows the day, the early moments of the match had already decided the champs, as the Rangers kept things under control with early goals. With a fantastic display of goal-keeping from Subhasish and compact defense from Surajit and Suman Ghosh for the Rangers it was hard for our strikers to evade their fort. Tushar da and Ganesh controlled the midfield well enough for the Rangers and assisted their striker Dilip to score a couple of hard fought bloodshedding goals to take them home with a 5-3 win in the final. With this, another session of fantastic footballing experience ends leaving behind a lot for us to cherish.

Photographs of SNB Football league are on the next page.

PHOTOGRAPHY

Sabyasachi Ghosh*Champion team**Snow covered Rohtang Pass**Runner up team*

CROSSWORD

Solution to Vol. 5, Issue: 3 Crossword

1	M	A	G	I	C		4	E	R	O	D	6	E
	O		A		U			M		B			V
	T		D		7	R	A	B	B	I			E
	I		G			L		R					N
8	F	R	E	E		9	C	Y	G	10	N	E	T
			T		11	A		O		U			
12	S	Y	S	T	E	M		13	A	C	I	14	D
	A					R		15	U		L		I
16	S	E	S	S	I	O	N			E			G
	I		E			A			I		A		I
17	N	O	W	E	L			17	T	A	R	O	T

**Satyendra Nath Bose National Centre for Basic Sciences**

Block-JD, Sector-III, Salt Lake

Kolkata - 700098

Editorial Board: J. Chakrabarti, R. K. Mitra, K. Acharyya, C. Biswas, M. Bose

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