



# Acharya Prafulla Chandra College

New Barrackpore, Kolkata - 700 131, West Bengal

(Govt. Sponsored | NAAC Accredited A Grade College with CGPA 3.23)

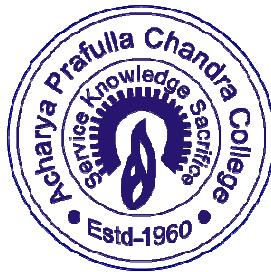
Department of Physics in collaboration with IQAC  
presents



Two Day National Level Seminar On  
**Recent Trends in Physics**  
**(RTP-2023)**

June 28<sup>th</sup> & 30<sup>th</sup>, 2023

# Book of Abstracts

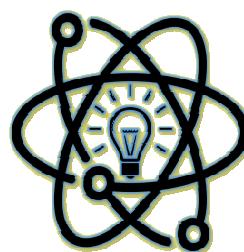


# **Acharya Prafulla Chandra College**

**New Barrackpore, Kolkata - 700131, West Bengal**

**Department of Physics in collaboration with IQAC**

**Presents**



**RTP-2023**

**Two Day National Level Seminar On  
Recent Trends in Physics  
(RTP-2023)**

**June 28<sup>th</sup> & 30<sup>th</sup>, 2023**

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## TWO DAYS NATIONAL LEVEL SEMINAR on RECENT TRENDS IN PHYSICS

**: Venue :**  
**Room No: DJB-4**  
**Acharya Prafulla Chandra College**

**Day 1        June 28, 2023**

<b>09:30 – 10:15</b>	<b>Registration</b>
<b>10:15 – 11:00</b>	<b>Inauguration &amp; Key-note Address</b>
<b>11:00 – 12:00</b>	<b>Invited Lecture I</b>  <b>Title</b> Mysteries of the Quantum World  <b>Speaker</b> <b>Dr. Ananda Dasgupta</b> Associate Professor, Dept. of Physics, IISER Kolkata.
<b>12:00 – 12:15</b>	<b>TEA BREAK</b>
<b>12:15 – 01:30</b>	<b>Oral Presentation (OP-01 - OP-05)</b>
<b>01:30 – 02:00</b>	<b>Special Lecture</b>  <b>Title</b> MEDICAL PHYSICS – Application of Physics in Medicine  <b>Speaker</b> <b>Dr. Apurba Kabasi</b> Consultant Medical Physicist, Medella Karkinos Oncology Institute. Topic: Medical Physics
<b>02:00 – 03:30</b>	<b>LUNCH &amp; Poster Presentation (PP-01 – PP-14)</b>
<b>03:30 – 04:30</b>	<b>Invited Lecture II</b>  <b>Title</b> Emergence of Dirac Materials in Carbon Family  <b>Speaker</b> <b>Dr. Debnarayan Jana</b> Professor, Dept. of Physics, University of Calcutta.
<b>4:30-05:00</b>	<b>Oral Presentation (OP-06 - OP-07)</b>



**Day 2         June 30, 2023**

**10:00-10:30**      Registration

**10:30 – 12:30**      **Invited Lecture III**

**Title**            The Fascinating Cosmos

**Speaker**          **Dr. D. P. Duari**

Former Director, M. P. Birla Institute of Fundamental Research, Kolkata

**12:30 – 12:45**      **TEA BREAK**

**12:45 – 02:00**      **Oral Presentation (OP-08- OP-12)**

**02:00 – 03:30**      **LUNCH & Poster Presentation (PP-15 – PP-28)**

**03:30 – 04:30**      **Invited Lecture IV**

**Title**            Thermodynamics for Small Systems

**Speaker**          **Dr. Sourabh Lahiri**

Assistant Professor, Dept. of Physics, BIT Mesra

**04:30**            Valedictory session and closure of the conference

Event website: <https://apccphysics.github.io/rtp2023>



## Content of Abstracts

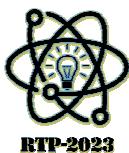
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### **Invited Lectures**

Mysteries of the Quantum World <i>Ananda Dasgupta</i>	IP-01
Emergence of Dirac Materials in Carbon Family <i>Debnarayan Jana</i>	IP-02
The Fascinating Cosmos <i>D. P. Duari</i>	IP-03
Thermodynamics for small systems <i>Sourabh Lahiri</i>	IP-04

### **Oral Presentation**

Construction of Rotation Curve of the Milky Way from Disk and Non-disk tracers <i>Pijushpani Bhattacharjee, Soumini Chaudhury, Susmita Kundu</i>	OP-01
$\beta^-$ Decay of Bare Atoms in Stellar s-Process Environments <i>Arkabrata Gupta, Chirashree Lahiri, and S. Sarkar</i>	OP-02
Information theoretic measures of one-electron quantum dot <i>Santanu Mondal, A. K. Roy, J. K. Saha</i>	OP-03
Efficient two-dimensional localization of Rubidium Rydberg atom using probe absorption in a microwave-driven five-level system and its application as a phase-diffraction cross-grating <i>Aparajita Das, Md. Mabud Hossain, Jayanta K. Saha</i>	OP-04
Construction of Coherent-State Structure for Position Dependent Effective Mass Hamiltonian <i>Kalpana Biswas</i>	OP-05
On the generalized Peres-Horodecki separability in noncommutative space <i>Pinaki Patra</i>	OP-06
Isolating noise and amplifying signal with quantum Cheshire cat <i>Ahana Ghoshal, Soham Sau, Debmalya Das, Ujjwal Sen</i>	OP-07
All Optical Filter Design using Photonic Crystal <i>Arpan Deyasi</i>	OP-08
Competitions between normal cationic order versus La-O covalency effect determines the Half metallic Antiferromagnetic (HM-AFM) Character in LaA(Ca/Ba)VMoO <sub>6</sub> double perovskites <i>Swarup Kumar Neogi, Abhisek Bandyopadhyay, Atanu Paul, Indra Dasgupta, Sudipta Bandyopadhyay, Sugata Ray</i>	OP-09



Comparative study of different phenomenological models to calculate $\alpha$ -decay half-lives <i>Writam Sengupta, Arkabrata Gupta</i>	OP-10
Computational Study on the Catalytic Role of Pincer Ruthenium(II)- PNP Complex in Directly Synthesizing Ester from Primary Alcohol <i>Suniti Ghosh, Rama Rathi, Abhijit K.Das</i>	OP-11
Quantum Key Distribution <i>Arnab Halder</i>	OP-12

## Poster Presentation

Entangled Su-Schrieffer-Heeger Chains: Flat bands and Topological Issues <i>Sauvik Chatterjee, Sougata Biswas</i>	PP-01
Three dimensional quantitative structure activity relationship and molecular docking studies of flavonoids as reverse transcriptase inhibitors <i>Bikash Kumar Sarkar and Nabanita Giri</i>	PP-02
The magnetic study of Cu doped ZnO: Theoretical approach <i>Apurba Kumar Nayek, Bidyut Halder, Dirtha Sanyal, Mahuya Chakrabarti</i>	PP-03
Determination of activation energy and order of kinetics of thermoluminescence peaks recorded with hyperbolic heating profile <i>Siddhartha Bhattacharjya, Shriparna Roy, I. Bhattacharyya, P. S. Majumdar</i>	PP-04
Structure and stability of nitriles and their iso-nitriles ( $\text{CH}_3\text{CN}$ ; $\text{CH}_3\text{NC}$ , $\text{CH}_2=\text{CHCN}$ ; $\text{CH}_2=\text{CHNC}$ and $\text{CH}_3\text{CH}_2\text{CN}$ ; $\text{CH}_3\text{CH}_2\text{NC}$ ): A theoretical study <i>Shriparna Roy, Siddhartha Bhattacharjya, I. Bhattacharyya, Narayan C. Bera</i>	PP-05
Orienting discotic liquid crystal in an innovative method <i>Surjya Sarathi Bhattacharyya and Yves Galerne</i>	PP-06
Study of charged bodies in Modified Gravity <i>Aritra Sanyal</i>	PP-07
Monte-Carlo simulation to study a liquid like system <i>Amiya Mondal</i>	PP-08
Hydrofuel – A future source of energy <i>Sneha Das, Debraj Adhikary</i>	PP-09
Distinction Between Classical Point of View & Quantum Point of View <i>Ritam Mahanta, Sauptik Sadhukhan</i>	PP-10
Solving Bernoulli's Equation by Variable Separation <i>Upamanyu Ghose</i>	PP-11
Bound and Resonance ${}^3\text{Fe}$ States of Helium Atom under Plasma Confinement <i>A. N. Sil, S. Dutta, D. Ghosh, J. K. Saha, S. Bhattacharyya, T. K. Mukherjee</i>	PP-12
Dielectric Properties of ZnTe Nanomaterial <i>Ayshwarya Saha</i>	PP-13
A brief review on smart materials <i>Agniva Paul and Rajkumar Singha</i>	PP-14



Recent Advancements in Blood Glucose MonitoringTechnology <i>Mahua Karmakar</i>	PP-15
Layer- by- layer electrostatic self assembled film of anionic dye sulforhodamine B and a cationic bio polymer Poly-L-Lysin: A spectroscopic and Atomic force microscopy study <i>Alapan Pal, Pabitra Kumar Paul</i>	PP-16
Magnetosonic Shocks and Solitons in Fermi Plasma with Quasiperiodic Perturbation <i>Sharry, D. Dutta, M. Ghosh and S.Chandra</i>	PP-17
Characteristics of isotherm and Schottky diode of lead (II) iodide coordinated azo-imidazole by Langmuir-Blodgett technique <i>Ujjal Saren, Pabitra Kumar Paul</i>	PP-18
Fabrication of multifunctional PVDF/rGo Composites and their enhanced dielectric properties. <i>Jweel Mazumder, Dr. Debabrata Bhadra</i>	PP-19
Preparation of PVDF/GO nanocomposite films exhibiting largely enhanced dielectric properties <i>Susmita Das, Jweel Mazumder, Dr. Debabrata Bhadra</i>	PP-20
Influence of water sorption on ionic conduction of polymer composite film <i>Anamika Das, Satarupa Biswas, Madhumita Mukhopadhyay</i>	PP-21
s-, p- & d- wave phase shifts in Ps – He scattering using a Static Exchange Model <i>Nirmal K. Sarkar</i>	PP-22
Viscosity of Ethylene Glycol (EG) base fluids containing Graphene Nanosheets (GNS): Insight from Molecular Dynamics <i>Sakti Pada Shit</i>	PP-23
Crystal Structure of 3-phenylsulfoxy coumarin derivatives <i>Goutam Biswas</i>	PP-24
Theoretical study on structure, dissociation pathways and thermochemical analysis of R-CN (R= CH <sub>3</sub> -, CH <sub>2</sub> CH-, CH <sub>3</sub> CH <sub>2</sub> -) molecules <i>Shriparna Roy, Siddhartha Bhattacharjya, Narayan C. Bera and Indranil Bhattacharyya</i>	PP-25
Evaluation of the activation energy of thermal peaks recorded under quadratic heating scheme without prior knowledge of order of kinetics <i>Siddhartha Bhattacharjya, Shriparna Roy, I. Bhattacharyya and P. S. Majumdar</i>	PP-26
Analyzing the Generalized Coherent States for Free Particles <i>Muklesur Rahaman, Shilpa Nandi, Pinaki Patra</i>	PP-27
Synthesis of Ni(OH) <sub>2</sub> nano powder by electrolyzing mechanism and investigation ofphotocatalytic and supercapacitorproperties <i>F.E.Aman and S. K. Pradhan</i>	PP-28



## Invited Scientific Articles

MEDICAL PHYSICS – Application of Physics in Medicine <i>Apurba Kabasi</i>	IA-01
What are nanomaterials, and how do we characterize them? <i>Pralay K. Santra</i>	IA-02
Nuclear magnetic resonance spectroscopy in materials research <i>Bilwadal Bandyopadhyay</i>	IA-03
Applications of Computational Methods to Physics and Chemistry <i>Abhijit Kumar Das</i>	IA-04
Macromolecular X-ray Crystallography and Use of Synchrotron Radiation <i>Goutam Biswas</i>	IA-05



## Aim of the Seminar

This seminar aims to provide a dynamic platform for students and teachers to gain exposure to different areas of physics. In students, this will hopefully enhance the love for physics. They will get to know what leading researchers do with their training in physics. During the talks, they may be able connect various topics from their syllabus to the topics discussed in the talks. For teachers and researchers, this will give ideas about different areas to explore in their research. They may also get ideas about ways to solve their research problems, that are different from the traditional approaches in their research area. This will also be a platform for similar minded people to discuss and exchange ideas.

## Scope of the Seminar

This seminar will cover topics covering areas in condensed matter theory, general relativity, mathematical physics, non-equilibrium statistical physics, astronomy and astrophysics. In addition, there will be contributed talks covering other areas of physics. If you are a person who liked your science subjects when you were in school, then this seminar is for you. If you like to watch sci-fi movies, then this is for you. If you are stuck at your research problem and looking for a new idea which can disentangle your thought process, then this is for you. If you are an open minded scientist who finds all areas of science interesting, then this is for you. Our invited speakers have promised to deliver lectures which should be at a colloquial level and should be interesting to anyone who is interested in science, mathematics or logical reasoning.

Our first invited speaker, Dr. Ananda Dasgupta, will give you a glimpse of quantum mechanics and tell you the importance of the most recent Nobel Prize in physics. Our next speaker, Dr. Debnarayan Jana, will talk about topics in Condensed Matter Physics and introduce Dirac materials. Your mathematics teacher in school may have taught you that functions are typically parabolic at their minima and maxima. Dirac materials serve as a counter example, where hills and valleys look conical (linear) near their peaks and bottoms. You may have also heard in school that entropy always increases. Our third speaker, Dr. Sourabh Lahiri, will convince you that this need not always be true. Our final speaker, Dr. Debiprosad Duari, will take you to the skies and give you a tour of stars, galaxies, planets, black holes and leave you with lots of beautiful pictures to dream about. Participants will leave with a flavour of a vast array of ideas and information in physics for future study and research.



## About the Department

*“The aim of Science is not to open the door to infinite wisdom, but to set a limit to infinite error.”*

Bertolt Brecht

The Department of Physics began its journey in the year 1961 when the college was affiliated under the University of Calcutta. Back then, the college only offered Pre University and B.Sc. General Course to the enrolled students. The prestigious moment for the Department came in the year 1994 when Honours Course was introduced. The Post Graduation course in Physics was introduced in the year of 2009. Presently the Department offers both Honours, General courses along with the Post Graduation Course under the curriculum of the West Bengal State University.

At the age of digitalization, the literary corpus is always scanned and placed online. It has been difficult to teach in such an age when there is an abundance of materials available online. So, we primarily stick to the traditional teaching method of Chalk and Talk", Our first duty is to tell the students how to identify the authentic problems, processing and reading. It is a constant challenge to keep the students stuck to the text books along with exposing them to the growing boundaries of the ever increasing digital empire. The same constraint is identified and accepted by us and we are in a constant process of evolving new methods where the students would choose the physical library over the virtual one.

Our mission, besides class-room teaching, is to attain a holistic development of our students, where they would not only be literary competent, but also socially aware of the environment around them. Our Department is like the second home for both the learners and the facilitators, where we walk hand in hand dreaming together of a creative haven.

The faculty and the alumni of the Department always encourage our present students, who mostly are first generation learners and come from economically challenged background, to expand the limits of their creative inspirations. We arrange workshops, seminars, special lectures, academic exchange programmes, cultural gatherings, tutorial and remedial classes, internal evaluations, parent-teacher meetings, publishing wall-magazines and departmental journals to cater the both academic and non-academic needs of the students.

However, we try to offer our best efforts and prepare our students to meet up challenges of global competition and strive towards perfection.



## Message from the Desk of TIC

Dr. Syed Rafi Ahmed

The Department of Physics in collaboration with Internal Quality Assurance Cell (IQAC) of Acharya Prafulla Chandra College, Kolkata-700131 has taken an ambitious program to organise a two days National Level Seminar on Recent Trends in Physics (RTP-2023).

The two days seminar will cover topics on condensed matter theory, quantum mechanics, mathematical physics, non-equilibrium statistical physics, astronomy and astrophysics. It will cover keynote address, invited talk from the eminent academicians, poster presentation and other events. I hope two days (28th and 30th June 2023) deliberations and meaningful interaction among the experts and participants will be immensely helpful for the entire fraternity and will emerge commendable creative ideas and knowledge through mutual discussions.

On this occasion I convey my best wishes to the entire Physics Department of the college for their relentless endeavour in making the seminar a grand success.



## Message from the Ex-Principal

Dr. Saktibrata Bhowmik

It gave me immense pleasure to note that the department of Physics in collaboration with the IQAC of the college is organizing a two-day national seminar on Recent Trends in Physics (RTP 2023) on 28<sup>th</sup> and 30<sup>th</sup> June 2023.

The objective of this seminar is to have a greater understanding of physics and to provide a dynamic platform for students and teachers to gain exposure to different areas of physics both in teaching- learning and research.

Department of Physics in the college is one of the departments which offers Post Graduate course since 2009. A large number of students have passed out successfully from this department and are well placed in different positions in the society. A considerable number of students passing out from this department are engaged in active research in different institutions of national and international repute. Teachers in the departments are also involved in active research and have published high quality research articles in different national and international journals. Some teachers in the department have supervised and supervising research scholars leading to Ph.D degree. It is worth mentioning that an ex-teacher of the department was awarded Ph.D degree doing research in the department under the supervision of another teacher in this department.

I am confident that through the deliberations of the eminent speakers , share and exchange of ideas and information on the topic , the seminar will help the students as well as the faculty members for a greater understanding on the Recent Trends in Physics and will focus on different areas to explore research.

I would like to convey my thanks to the organizers for taking such initiative and wish a grand success of the seminar and at the same time I hope that the department of Physics will move forward excelling further both in teaching- learning and research to accomplish its goal.



## Message from the Desk of Convener

Dr.Indranil Bhattacharyya

Dear esteemed participants,

On behalf of the organizing committee, it is with great pleasure that I extend my warmest wishes to all of you attending the seminar “Recent Trends in Physics (RTP-2023)”. In this enlightening event, I am truly honoured to have such a distinguished gathering of brilliant minds and accomplished researchers in their respective fields.

The realm of physics is a dynamic and ever-evolving discipline, and it is through the enlightening events like seminar where we can assemble ourselves together to share our knowledge, exchange ideas, and foster collaboration.

Our focus on recent trends in physics reflects the rapid progress made in the field over the past few years. From the astonishing advancements in quantum information and computing to groundbreaking discoveries in multifarious domains of science have captivated our imaginations and expanded the frontiers of human understanding.

As we gather here, I encourage you all to embrace the spirit of intellectual curiosity and engage in lively discussions and debates. The power of collective thinking and the cross-pollination of ideas can lead to ground-breaking insights and novel approaches to tackling the most complex scientific challenges.

I do sincerely hope that this seminar serves as a catalyst for forging new connections and collaborations that will drive future research endeavours. Let us seize this opportunity to learn from one another, to foster interdisciplinary collaborations, and to inspire the next generation of physicists who will carry the torch of discovery forward.

Wishing you all a stimulating and rewarding seminar experience as well your contributions and discussions may pave the way for transformative advancements in the realm of physics.

With warm regards,



## Message from Prof Prasanta Kumar Mukherjee

School of Mathematical Sciences, RKMVERI, Belur Math

I am very happy to know that the Department of Physics of Acharya Prafulla Chandra College is going to organize a two-day national-level seminar by eminent physicists and presentation of the research activities of young researchers and students during 28 and 30<sup>th</sup> June, 2023. It is covering lectures on limited but important areas in contemporary Physics along with short oral and poster presentations by young researchers. Such an attempt is long overdue. It will not only give impetus to the students and research community a feeling about the current scenario but also encourages them to go forward in directions of frontier areas of research in physics. I wish you all from my heart a great success in the outcome of the given effort. I look forward for a sustained activity along this line in the days to come for the enhancement of knowledge in physics.



## *Invited Lectures*



IP-01

## Mysteries of the Quantum World

Ananda Dasgupta

Department of Physics, Indian Institute of Science Education and Research Kolkata

We will explore some of the puzzling features of the microworld. The list of quantum mysteries is really long - the superposition of states, wave particle duality, entanglement, and so on. With advances in modern technology, many of these mysteries are now within the reach of experimental verification. We will see how the underlying logic of the quantum world, while weird to our classical sense, does have an internal consistency of its own.

IP-02

## Emergence of Dirac Materials in Carbon Family

Debnarayan Jana

Department of Physics, University of Calcutta, Kolkata- 700009

E-mail:[djphy@caluniv.ac.in](mailto:djphy@caluniv.ac.in)

The physics of two dimensional (2D) materials is always intriguing in their own right. Dirac materials are a class of complex and functional nanomaterials offering great potential in the development of new electronic components. In this talk, we would like to present some theoretical calculations of electronic properties of graphene, S-graphene, phagraphene, and 8-16-4 Graphyne systems. A tight binding (TB) model along with density functional theory (DFT) will be used to unravel the characteristic features of Dirac points in these systems. Further, we will discuss an analytical scheme to address the emergence and robustness of Dirac fermions in phagraphene network. All these theoretical results in non-honeycomb structure may shed light on device fabrication in nano opto-electronic technology and materials characterization techniques in 2d carbon allotropes.

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- 3 S. Jana, A Bandyopadhyay, D. Jana, Phys. Chem. Chem. Phys., **10**, 1039 (2019).
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9. A. Bandyopadhyay and D. Jana, Rep. Prog. Phys., **83**, 056501 (2020).
10. O. Vafek, A. Vishwanath, Annu. Rev. Condens. Matter Phys. **5**, 83 (2014).
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12. M. Ghosh, A. Bandyopadhyay, Suman Chowdhury and D. Jana, Appl. Surf. Science, **577**, 151782 (2022).

IP-03

## The Fascinating Cosmos

Dr. Debiprosad Duari

Former Director, M. P. Birla Institute of Fundamental Research, Kolkata

The subject of Astronomy is considered to be the oldest subject that was practised and learnt by ancient people. Amazingly, it is also the most recent subject of interest and scientific research as well. Scientists all over the world, have realised that terrestrial laboratories have their own limitations in verifying the different hypothesis that the scientists put forward in their endeavour to formulate physical laws which governs the nature. They have realised that it is in the vast expanse of fathomless space, among the multitudes of stars, within the confines of billions of galaxies, considering the universe as a single system, the secrets of nature, the profound yet simple physical laws governing it possibly can be discovered. It is with this great promise that Astronomy has become an extremely important and well sought after subject among the scientists and academic minded people.

In the lecture, we will try to go through a snapshot survey, first on our neighbourhood – the solar system and neighbouring stars. With technological developments, newer and more complex, efficient telescopes have been built recently, spacecrafts with various detectors have been sent to the planets and some of their satellites in the last three decades, and they have unearthed a vast amount of knowledge about our own Solar system, which earlier people could only imagine. Moreover, the realization that the presence of life on earth and the environment conducive for supporting life is a result of a series of chance happenings which shaped and evolved the earth, its atmosphere and especially the physical and chemical characteristics which allowed the evolutionary processes to arrive at the present world that we live in.

The birth, evolution and the present status of the solar system which originated around 4.6 billion years from a cloud of gas and dust will be discussed along with the new bodies that have been discovered recently. Each planet especially Mars will be discussed in details for the recent interest of having water and subsequently habitation in the planet. The knowledge of the Solar System consisting of Sun and nine planets have been drastically revised by new observations and theoretical understanding about it. At present the Solar system is characterized not only by the planets, but the property of their satellites, thousands of space debris called asteroids, mostly circling the Sun between the orbit of Mars and Jupiter. Some of the asteroids have the potential to collide with the earth resulting in destruction of life and property as probably had happened earlier. A new class of objects newly named as Dwarf Planets of which Pluto has been made a member will be touched upon in the discussion. The search for liquid water and any markers of life in our solar system have interested the scientists and common people for long. Recent advances on these issues will also be discussed.



A brief outline of stellar birth, evolution, death of small, intermediate and massive stars will be discussed. In the course of our discussion about stars and their evolution and properties, the birth of a star from interstellar giant molecular clouds and the end phase of stars are probably most exciting story of our universe. The death of low mass stars resulting in Red Giant, Planetary Nebula and White dwarf. Medium mass stars at their end phase after producing iron at its core goes through a core collapse ultimately resulting in an explosive event called Supernova. The remnant becomes a neutron stars, and if it spins becomes a pulsar. The nucleosynthesis of elements that goes on inside the star is the only process in the universe to produce elements other than hydrogen and helium which are thought to be formed at the very early stage of the Universe. The Cosmic consciousness about everything that we see around and within us makes us realize that we are all star children. This almost philosophical yet realistic perception is one of the interesting aspect of the subject of Astronomy and Astrophysics. Next comes the end phase of large mass stars, who after their nuclear burning phase, because of their mass collapses into a singularity and are termed as Black Holes. The ever enigmatic black holes and their properties and new discoveries will be touched upon. How physical and chemical processes in stars shape our cosmic environment and even us, will be the highlight of the deliberation.

A very brief outline of our present understanding of the origin, evolution and present structure of the universe will be given to enthuse and excite young minds about the vast repository of Cosmic knowledge that has become apparent more so with the technological developments of astronomical instruments.



IP-04

## Thermodynamics for small systems

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Thermodynamics for small systems, typically called "Stochastic Thermodynamics", differs substantially from that of macroscopic ones, due to the significant effect of thermal noise on the dynamics. The various observables appearing in stochastic thermodynamics are defined as per the standard prescription provided by Ken Sekimoto more than two decades ago. These definitions are of paramount importance to scientists in the studies of small-scale devices like microscopic heat engines or refrigerators. Furthermore, there exist relations valid under very general assumptions, that give rise to the Second Law of Thermodynamics as a corollary.



## *Oral Presentation*

OP-01

# Construction of Rotation Curve of the Milky Way from Disk and Non-disk tracers

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The rotation curve (RC) of our Galaxy, the Milky Way, is constructed starting from its very inner regions (few hundred pc) out to a large Galactocentric distance of  $\square 200$  kpc using kinematical data on a variety of tracer objects moving in the gravitational potential of the Galaxy, without assuming any theoretical models of the visible and dark matter components of the Galaxy. We study the effect on the RC due to the uncertainties in the values of the Galactic Constants (GCs)  $R_\odot$  and  $V_\odot$  (these being the sun's distance from and circular rotation speed around the Galactic center, respectively) and the velocity anisotropy parameter  $\beta$  of the halo tracer objects used for deriving the RC at large Galactocentric distances. The resulting RC in the disk region is found to depend significantly on the choice of the GCs, while the dominant uncertainty in the RC at large distances beyond the stellar disk comes from the uncertainty in the value of  $\beta$ . In general we find that the mean RC steadily declines at distances beyond  $\square 60$  kpc, independently of the value of  $\beta$ . Also, at a given radius, the circular speed is lower for larger values of  $\beta$  (i.e., for more radially biased velocity anisotropy). Considering that the largest possible value of  $\beta$  is unity, which corresponds to stellar orbits being purely radial, our results for the case of  $\beta=1$  give a lower limit to the total mass of the Galaxy within  $\square 200$  kpc,  $M(200 \text{ kpc}) \geq (6.8 \pm 4.1) \times 10^{11} M_\odot$  independently of any model of the dark matter halo of the Galaxy.



## $\beta^-$ Decay of Bare Atoms in Stellar s-Process Environments

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In stellar s-process environments (Temperature  $T \sim 10^8$  K –  $5 \times 10^8$  K, free electron density  $n_e \sim 10^{26}/\text{cm}^3 - 10^{27}/\text{cm}^3$ ) it is possible that even the high Z elements are partially or fully ionized. In this situation,  $\beta^-$  decay to the continuum is not the sole option. Due to the availability of unoccupied atomic orbits,  $\beta^-$  decay to the atomic bound state becomes another probable channel. Moreover, at these temperatures, low-lying excited energy levels of the parent nuclei may have thermal equilibrium population, and those excited levels may also decay via  $\beta^-$  emission. In this work, we have presented allowed  $\beta^-$  decay rates to the continuum and bound state of a few s-process nuclei in the mass range  $A = 60 - 80$ , from the ground/ isomeric nuclear states of the parent. The presence of bare atoms in these situations has been confirmed by solving the Saha ionization equation. The ratio of bound to continuum decay rates has been calculated as a function of  $\beta^-$  decay Q value. Finally, we have compared the total  $\beta^-$  decay half-life (due to  $\beta^-$  decay to bound state and continuum state) of the bare atoms in stellar conditions with their terrestrial  $\beta^-$  decay half-life. In most of the cases, it has been observed that the stellar  $\beta^-$  decay half-life becomes shorter than the terrestrial half-life due to the presence of bound state  $\beta^-$  decay. These results are useful for s-process nucleosynthesis calculations.

## Information theoretic measures of one-electron quantum dot

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Confined quantum system emerges as one of the most important tools to determine the characteristic behaviour of a quantum system in the laboratory environment. Researchers use various kind of model potentials to simulate different confining conditions. For instance, in case of hard and soft type spatial confinement, spherical cavity, spherical shell, finite oscillator, harmonic, rectangular, parabolic, Woods-Saxon, Poschl-Teller, Rosen-Morse, Tietz, and Eckart etc. are some of the potentials [1] widely used for such purpose. In this regard, the study on quantum system in quantum dot (QD) environment mimicked by finite oscillator (FO) potential has gained considerable momentum as the experimental simulation of such confining environment is now available in the laboratory. Moreover, such investigation has a wide range of applications in biotechnology, modelling molecules with tunable bonds, semiconductors, LEDs, transistors, diode lasers, solar cells, and medical imaging etc. [2].

Recent years have witness an overwhelming interest to researchers in different branches of science on the information measures for spatially confined quantum system [3]. This is because of the tunability of the information content in the quantum system by solely manipulating the confinements parameters. In atomic system, the localization or de-localization of electronic charge distribution is estimated through information measures. Shannon entropy and Fisher entropy are mostly used information measures and frequently arises in the study of quantum information theory, quantum computing, quantum communication etc. [4].

In the present work, we have studied the variation of position and momentum space Shannon entropy, Fisher entropy, Fisher-Shannon complexity and related inequalities corresponding to the ground and different low-lying excited states of H atom under the effect of FO potential. The H atom under FO potential may alternatively be treated as an one-electron QD with attractive Coulomb impurity at the centre. Therefore, by tuning the cavity parameters (width and depth), we have estimated the above mentioned information measures. It has been noted that within the approximate limit of width of potential 10 a.u. to 100 a.u., all the information contents are modified significantly, whereas change in the depth of the potential can only further enhance those quantum information measures.



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# Efficient two-dimensional localization of Rubidium Rydberg atom using probe absorption in a microwave-driven five-level system and its application as a phase-diffraction cross-grating

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Quantum coherence based precision position measurement of moving atoms and its localization in space have been a longstanding issue for the researchers. The main difficulty in the position measurement was its highest possible accuracy which is restricted by the Heisenberg uncertainty principle. Irrespective of the prevailing difficulties in the measurement of atom position with high-precision, a variety of its applications *e.g.* laser cooling and trapping of neutral atoms [1], atom nanolithography [2], measurement of the center-of-mass wave function of moving atoms [3] *etc.* attracted much attention of different research groups. However, the advent of quantum optics has impressively reshaped the techniques for precision position measurement of atom over the past few years. Localization of atom in one-dimensional (1D) [4], two-dimensional (2D) [5] and three-dimensional (3D) [6] space by means of probe absorption in coherently prepared atomic medium is one of them.

We have proposed a microwave mediated 2D atom localization scheme involving Rydberg states. The localization of atoms are realized in terms of the absorption of the optical probe field that connects the ground state with a four-level diamond-like closed-loop formed by two pump fields (producing mutually orthogonal standing-waves) and two microwave fields (which are running waves) driven atomic transitions. It is observed that the probe laser is absorbed by the cold atoms in 2D plane which forms parallel line, wave-like line, elliptical- and lattice-like patterns. These patterns signify atom localization in 2D space. The influence of probe detuning, microwave field strength ratios and relative phase between them, dipole-dipole interaction between the atoms in the Rydberg states on the atom localization are explored. The pump strength to microwave strength ratios corresponding to the two atomic transition branches, configuring the diamond-like closed-loop is found to affect the localization pattern for different relative phases. Interestingly, the strength ratios of the pump and microwave fields follow a balancing condition when discrete lattice-like patterns



appear. This balancing condition is similar to the Wheatstone bridge balance condition for the electrical circuit. A possible application of the five-level system as a phase-diffraction cross-grating is presented by examining the variation of first-order diffraction intensity *w.r.t.* the probe detuning and the two microwave field strength ratios.

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## Construction of Coherent-State Structure for Position Dependent Effective Mass Hamiltonian

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Being the minimum uncertainty state, the coherent state structure might be helpful for the bridging between classical and quantum mechanics. Due to the non-commutativity of position and momentum, the viable form of quantum Hamiltonian regarding position dependent effective mass (PDEM) is a controversial issue. To encounter this issue, the kinetic part for PDEM Hamiltonian is derived from the first principal.

We have advocated our starting point of construction of the Hamiltonian by considering the combination of positions and momentums from classical level of calculation. Then, the coherent state structure for PDEM Hamiltonian has been constructed by using the algorithm of supersymmetric (SUSY) quantum mechanics.



## On the generalized Peres-Horodecki separability in noncommutative space

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With the help of the generalized Peres-Horodecki separability criterion (Simon's condition) for bipartite Gaussian state, we have studied the separability of the noncommutative space (NCS) coordinate degrees of freedom. Non-symplectic nature of the transformation between the usual commutative space and NCS restricts the straightforward use of Simon's condition in NCS. We have transformed the NCS system to an equivalent Hamiltonian in commutative space through the Bopp shift, which enables the utilization of the separability criterion. To make our study fairly general and to analyze the effect of parameters on the separability of bipartite state in NC-space, we have considered a bilinear Hamiltonian with time-dependent (TD) parameters, along with a TD external interaction, which is linear in field modes. The system is transformed into canonical form keeping the intrinsic symplectic structure intact. The solution of the TD-Schroedinger equation is obtained with the help of the Lewis-Riesenfeld invariant method (LRIM). Expectation values of the observables (thus the covariance matrix) are constructed from the states obtained from LRIM. It turns out that the existence of the anisotropy in the oscillator determines the separability of the states. In particular, for an isotropic oscillator, the bipartite states are always separable, whereas a particular anisotropic parameter value may cease the separability. With the help of a toy model, we have demonstrated how the tuning of a TD-NCS parameter affects the separability.



## Isolating noise and amplifying signal with quantum Cheshire cat

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The so-called quantum Cheshire cat is a phenomenon in which a property of an object that is associated with a "cat" and a "grin" on the cat are separated. We suggest a thought experiment using an interferometric setup that is analogous to this phenomenon, in which a property (a component of polarization) of an object (a photon) can be separated from the object itself and simultaneously amplified when it is already decoupled from its object. We also demonstrate how this configuration can be used to separate two complementary properties, such as two orthogonal photon polarization components associated with a cat's grin and snarl, from one another so that one of them can be amplified while being separated from the other. Furthermore, we extend the work to a noisy scenario where the object is identified as a so-called confused Cheshire cat and is affected by an additional interaction term that is similar to spin-orbit coupling in the Hamiltonian for the measurement process. We create a thought experiment where a "confusion" of this nature can be successfully separated from the system, and we discover that the separation aids in signal amplification.

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# All Optical Filter Design using Photonic Crystal

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One of the key building blocks in the world of modern photonic integrated circuit is photonic crystal, which has already demonstrated superior qualities to those of its traditional counterparts in realizing optical devices. A periodic arrangement of dielectric materials, it efficiently controls the localization of electromagnetic waves [1] that are propagating inside the structure by adjusting certain structural parameters. This is made feasible by the development of photonic bandgap, a characteristic that is widely utilized to create photonic integrated circuits [2], transmitters, receivers, photonic crystal fiber, quantum information processing etc. For effective communication, this innovative microstructure has replaced traditional optical fiber.

It has been indicated that only 1D and 2D structures are effective to realize experimentally and for implementation purposes in various optoelectronic integrated circuits out of the many types of confinements that have been taken into consideration for photonic crystal analysis. In addition to the well-known metal-dielectric or dielectric stacks, a number of materials, including negative index materials, are suggested for the construction of PhC-based filters. Metamaterials, more precisely materials with a double-negative refractive index, are already used to boost SNR in antenna systems, preferably in those with active components that operate in the high frequency range. Thus, a unique approach of optical filter design with improved noise immunity results from the integration of an appropriate metamaterial structure into a 1D photonic crystal. Recent research has examined the transmission characteristics of photonic crystals based on metamaterials.

To choose the desired spectral range, defect-based structures are examined [3]. Investigation reveals how changes in incidence angle, metamaterial length, and air thickness affect an optical filter's transmission properties. Due to the fluctuation of these parameters for the TE and TM modes as well as bandwidth variation, transmission qualities have been examined. Based on these findings, researchers suggest optimum design for appropriate filter performance with specific percentage of point defect, intentionally invoked that enhance the filter action.

Compared to binary designs, ternary photonic crystals offer superior slope in the desired frequency range and less ripple in the passband region. The construction will undoubtedly result in the practical realization of a photonic integrated circuit for almost noise-free information processing.



RTP-2023

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# Competitions between normal cationic order versus La-O covalency effect determines the Half metallic Antiferromagnetic (HM-AFM) Character in LaA(Ca/Ba)VMoO<sub>6</sub> double perovskites

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Study of Half metallic (HM) magnets have received enormous attention because of their potential applications in spintronics and related fields [1-2]. These magnets are showing high degree of spin polarization of the charge carriers, due to by the half metallic character [3]. Half metallic antiferromagnets (HM-AFM) are another important class of Half metallic (HM) magnets in which the total integral magnetic moment is zero [4-5]. The present work demonstrates structural and physical property studies of double perovskite (DP) LaAVMoO<sub>6</sub>(A= Ca<sup>2+</sup>, Ba<sup>2+</sup>; abbreviated as LCVMO and LBVMO) compounds as possible half metallic antiferromagnet (HM-AFM) candidates [4-5]. In case of LCVMO with DP structure, La-O covalency brings forth strong competition against normal cationic order and thereby producing unusual phase-separation within the structure. It is evident that Ca<sup>2+</sup> and Ba<sup>2+</sup> at the A-site would offer a tool to modify the A-site ordering and thereby manipulating La-O covalency. Our experimental results reveal that LCVMO sits at the extreme end of phase separation among the LaAVMoO<sub>6</sub>(A= Ca<sup>2+</sup>, Sr<sup>2+</sup>, Ba<sup>2+</sup>) DP family forming large volumes of La, V and Ca, Mo-rich phases, which finally accounts for all unusual magnetic properties of LCVMO [5]. On the other hand, LBVMO does not endorse such phase separation and maintains chemical homogeneity more or less. Hence LBVMO compound is more correctly described as a layered A-site ordered and nearly complete B-site disordered double perovskite. Further we did EXAFS analysis for these LCVMO and LBVMO samples. It confirms that the energy stability, gained by typical La-O covalency, leads to the preferential La, V and Ca,



Mo ionic proximity in LCVMO. On the other hand, it has been observed for LBVMO, A-site ordering is robust as ionic radii of Ba<sup>2+</sup> (1.61 Å) is much larger than La<sup>3+</sup> (1.36 Å). Substitution of La<sup>3+</sup> by divalent cations with comparable and much larger ionic radii (Ca<sup>2+</sup> and Ba<sup>2+</sup>, respectively) is to tune the interplay between site-ordering and La-O covalency effect in LCVMO and LBVMO samples [5].

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## Comparative study of different phenomenological models to calculate $\alpha$ -decay half-lives

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The  $\alpha$ -decay is a process through which an unstable parent nucleus spontaneously transforms into a more stable daughter nucleus by emitting a  $^4_2\text{He}$  nucleus ( $\alpha$ -particle). It is energetically favourable for these nuclides to decay by emitting  $\alpha$ -particles as they generally reside in heavy nuclide region ( $Z > 82$  &  $N > 126$ ) which is mostly devoid of any stable nuclides. The half-lives of such nuclides can be estimated using phenomenological models which mainly depend on factors like preformation and tunnelling probability of the  $\alpha$ -particle. This was originally shown by Gamow *et al.* in 1928 where they used ‘Quantum Mechanical Tunnelling Theory’ to predict the half-lives. Till date fundamental research has produced many such half-life prediction models with improved accuracies within different mass regions. But greater hindrance in accuracy is observed in these models for odd-A and odd-odd nuclides due to the pairing effects in nuclear shell structure. This leads to a lack of a singular good prediction model which can produce  $\alpha$ -decay half-lives with an acceptable consistency for all types of nuclides over a wide mass region. In this work, the results of Unified Formula (D. Ni *et al.*, Physical Review C 78, 044310 (2008)), Analytic Formula (G. Royer, Nuclear Physics A 848(3-4) (2010)) and Two-Potential Model (X. Sun *et al.*, Physical Review C 93, 034316 (2016), and Physical Review C 95, 014319 (2017)) as phenomenological models have been studied. Furthermore, the consistency and viability of the Unified Formula, to be a good prediction model, has been checked against the results calculated by G. Royer and X. Sun *et al.* for a set of 131 nuclides with  $212 \leq A \leq 261$ . We have selected this mass region according to the overlap region of the masses used in the aforementioned papers.

# Computational Study on the Catalytic Role of Pincer Ruthenium(II)- PNP Complex in Directly Synthesizing Ester from Primary Alcohol

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Preparation of ester is one of the most important reactions in organic chemistry (1). The most traditional method of synthesis of ester involves the reaction of an carboxylic acid or its derivatives of acid chloride or acid anhydride with an alcohol in presence of Bronsted acids like HCl, NaHSO<sub>4</sub>, HBF<sub>4</sub>, H<sub>2</sub>SO<sub>4</sub>, H<sub>3</sub>PO<sub>4</sub>, AcOH etc (2). In recent years, dehydrogenative coupling of two alcohols to make ester in presence of different transition metal catalysts is becoming popular, as this process is quite simple and environment friendly than the conventional methods (3).

In the present venture, two equivalents of the primary alcohol, 3-oxa-butanol, are employed for the preparation of the ester, 2-methoxyethyl-2-methoxyacetate, which involves the release of two equivalents of H<sub>2</sub>. The reaction is carried out in presence of the Ru-PNP pincer complex, [RuCl{N(CH<sub>2</sub>CH<sub>2</sub>PMe<sub>2</sub>)<sub>2</sub>} as the catalyst.

The potential energy surface (PES) associated with the formation of ester along with hydrogen release in presence of the catalyst, is scanned at two different levels of theory, both in gas phase and solvent medium, in order to get a graphical idea of the pathway involved. The whole assisting phenomena of the catalyst in the solvent medium is also investigated through the implementation of CPCM, considering Tetrahydrofuran (THF) as the bulk solvent. The investigation is further extrapolated to two other isoelectronic PNP-pincer complexes, Rh(PNP<sup>+</sup>) and Os(PNP), as catalysts, and a comparative study among the three systems is brought under scanner by studying the catalytic efficiencies. To perform these studies, the rate determining step is identified in each case along with the rate determining intermediates and transition states.

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## Quantum Key Distribution

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Quantum Key Distribution (QKD) has emerged as a cutting-edge technology in the real time secure communication, utilizing the principles of quantum mechanics to establish cryptographic keys with unparalleled levels of security, providing a robust defence against eavesdropping and unethical hacking attempts.

At its core, QKD relies on the principles of quantum superposition and entanglement to ensure the secure exchange of cryptographic keys between communicating parties. Unlike classical cryptographic approaches like Public Key Cryptography (RSA or AES) that rely on computational complexity assumptions, QKD achieves security based on the fundamental laws of physics.

The fundamental idea behind QKD is to exploit the properties of quantum states, such as photons, to encode information in a way that any attempt to intercept or measure these states would be immediately detectable. The most widely used QKD protocol is the BB84 protocol, which involves the random generation and exchange of quantum bits (qubits) encoded in different quantum states.

The security of QKD lies in the fact that any attempt to measure the transmitted qubits inevitably disturbs their quantum states, introducing errors that can be detected by the legitimate parties. This allows the detection of eavesdroppers, ensuring the secrecy of the shared key.

QKD technology faces several implementation challenges, including the need for high-quality photon sources, efficient detectors, and low error rates. Overcoming these challenges has been a focus of ongoing research and development in the field.

QKD has the potential to revolutionize secure communication by providing a level of security that is resistant to advances in computational power, such as those posed by quantum computers. It holds promise for applications in areas such as financial transactions, government communications, satellite communications, military communications and data privacy.



Two Day National Level Seminar On *Recent Trends On Physics (RTP-2023)* on June 28<sup>th</sup> and 30<sup>th</sup>, 2023

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## *Poster Presentation*



# Entangled Su-Schrieffer-Heeger Chains: Flat bands and Topological Issues

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Flat bands and topological phase transition in a non-trivial extension of SSH-chains, where multiple chains are cross-linked via sites that are periodically placed on a chain, are explored. The cross-linking sites can have any value of the coordination number. The energy eigenvalues corresponding to the flat bands along with their degeneracy are extracted by real space decimation scheme. The topological phase transition is confirmed by the existence of quantized zak phase for all Bloch bands and edge states that are protected by chiral symmetry, consistent with the bulk-boundary correspondence. In addition to the edge states, the entangled SSH systems are shown to give rise to clusters of localized eigen states in the bulk of the system, in contrast to a purely one dimensional SSH system.

# Three dimensional quantitative structure activity relationship and molecular docking studies of flavonoids as reverse transcriptase inhibitors

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A set of 29 flavonoid molecules are used to generate comparative molecular field analysis (CoMFA) and comparative molecular similarity indices analysis (CoMSIA) models. The best CoMFA model showed a cross-validated correlation coefficient ( $q^2$ ) = 0.762, non-cross-validated correlation coefficient ( $r^2$ ) = 0.939, standard error of estimate ( $S$ ) = 0.038, and  $F$  = 396. And that for CoMSIA model were  $q^2$  = 0.758,  $r^2$  = 0.957,  $S$  = 0.063, and  $F$  = 236. The models show a high predictive ability, validated by 11 flavonoid molecules. The docking studies shows the hydrogen bonding interaction is mostly responsible for binding of the flavonoids molecules in the binding pocket of HIV 1-RT protein (3HVT.pdb).

**Keywords:** AMV-RT, Flavonoids, CoMFA, CoMSIA, Docking.



## The magnetic study of Cu doped ZnO: Theoretical approach

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Ab initio calculations in the framework of density functional theory have been performed to calculate the electronic properties of Cu-doped ZnO. When the Cu atom is doped at the cation site, it produces a significant magnetic moment along with a semimetallic behavior. The 3d orbital electrons of the dopant are the main source of magnetism along with the p-orbital electrons of the neighboring oxygen atoms.. A detailed spin-spin interaction study has resolved the anomaly of ferromagnetic and anti-ferromagnetic spin ordering in the Cu-doped ZnO system. Two Cu-dopants have been doped at different Zn-sites by varying the dopant distance. The ground state energy for each spin-ordered system has been calculated with the spin-polarized condition. Moreover, it has been shown that the magnetic ordering in the Cu-doped ZnO system is following the indirect exchange of the Ruderman-Kittel-Kasuya-Yosida (RKKY) model.

PACS: 71.15.Mb; 75.50.Pp; 61.72.-y

Key-words: Density functional theory; Magnetic semiconductors; Defects

## Determination of activation energy and order of kinetics of thermoluminescence peaks recorded with hyperbolic heating profile

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A set of expressions are presented for the evaluation of activation energy of thermoluminescence (TL) peaks recorded with hyperbolic heating profile. In the present work along with the conventional half intensity points the peak widths at signal levels equal to 0.8 and 0.95 of the peak height are chosen to reduce the effects of satellite peaks. A method of estimation of the order of kinetics of a TL peak by using its symmetry factor is also proposed. The present method has been applied to computer generated TL peaks and encouraging results have been obtained.

## Structure and stability of nitriles and their iso-nitriles ( $\text{CH}_3\text{CN}$ ; $\text{CH}_3\text{NC}$ , $\text{CH}_2=\text{CHCN}$ ; $\text{CH}_2=\text{CHNC}$ and $\text{CH}_3\text{CH}_2\text{CN}$ ; $\text{CH}_3\text{CH}_2\text{NC}$ ): A theoretical study

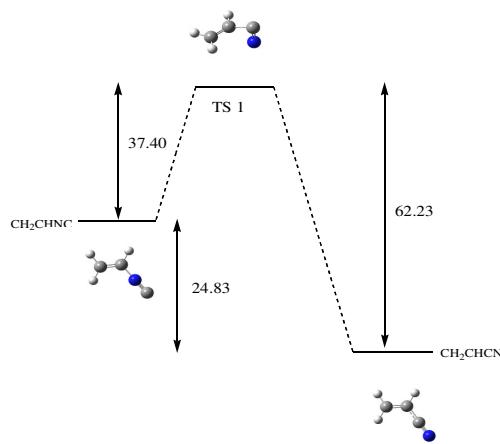
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Small nitriles are abundant in the interstellar region and the presence of *CN*-group acts as precursors of prebiotic substance. It is observed that the radiation environment such as *UV* radiation and ionization radiation process leads to different isomerization of molecules. The existence of acetonitrile ( $\text{CH}_3\text{CN}$ ), acrylonitrile ( $\text{CH}_2\text{CHCN}$ ) and propionitrile ( $\text{CH}_3\text{CH}_2\text{CN}$ ) and their iso-nitrile, isomers are detected in recent observation. In this study we have used density functional *B3LYP* method followed by high level ab-initio methods to study the relative stability and reaction pathways of small nitriles and their corresponding iso-nitriles substances. The nitriles are more stable compared to its isomeric form.



Schematic reaction diagram at MP2/cc-pVTZ level for the isomerization of  $\text{CH}_2\text{CHCN}$  to the corresponding  $\text{CH}_2\text{CHNC}$ . The relative energies are given in kcal/mol.

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## Orienting discotic liquid crystal in an innovative method

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The columnar liquid crystal phases are characterized by a partial translational ordering of the molecules into two dimensional arrays of flexible columns. It has already been exhibited by D. H. Van Winkle and N. A. Clark [1] that the discotic columns can be given a one-dimension freely-suspended structure with a diameter > 1  $\mu\text{m}$ , where the disk-shaped molecules are arranged into parallel columns. In the present paper we have investigated the alignment and morphology of freely suspended single discotic liquid crystal strands and then projected them over silanized glass plates. It has been observed that at high temperature the mesophase turned from columnar to nematic when weight fraction of the solvent was increased beyond a certain amount. Hence the addition of solvent in necessary proportion to the pristine columner liquid crystal host acts as lubricant between the columns.

Mixtures of Copper (II) dodecanoate and Triphenylene derivative with appropriate solvent concentration and appropriate temperature has been stretched in appropriate speed in order to generate single strands of diameter <1  $\mu\text{m}$ . They are then projected onto silanized glass plates. The strands have been characterized by polarized optical microscopy and atomic force microscopy. They are found to be stable in a well-aligned state for months while preserved at room temperature. In order to generate the thinnest possible strands, we have simultaneously controlled temperature, concentration of solvent, and pulling speed, which assists the thin one dimensional columnar strand fabrication. The shear induced stress over the disordered columnar phase on respective mixtures is responsible for the alignment. We have developed a new method for controlling the mentioned methodology which has potential application in the fabrication of new generation organic semiconductors.

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# Study of charged bodies in Modified Gravity

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This abstract explores various models and theories concerning the nature of the universe and introduces a novel perspective on charged ultra-dense strange quark stars based on modified  $f(R, T)$  gravity theory. Initially, Newton's static universe concept is discussed, where the isotropy and homogeneity of the universe suggest that matter is equally attracted in all directions. Einstein also supported a static universe filled with matter. However, W. de Sitter proposed a contrasting solution, considering a universe in motion without matter. The Friedmann model then describes an expanding universe, characterized by two independent Friedmann equations with an acceleration term indicating motion.

Building upon these foundational theories, this abstract presents a new model for charged ultra-dense strange quark stars using the modified  $f(R, T)$  gravity theory. The specific form of the  $f(R, T)$  function is simplified and explored in this context. Notably, this work represents the first instance, to the best of our knowledge, of a model for charged ultra-dense strange quark stars utilizing the modified  $f(R, T)$  gravity theory. The stellar structure is analyzed, and the effects of the modified gravity theory on the system are examined.

The abstract proceeds by introducing the Einstein-Maxwell field equation for the  $f(R, T)$  gravity theory and deriving the covariant divergence of the energy-momentum tensor. The assumption  $f(R, T) = R + 2\gamma T$  is made, allowing for a deeper investigation of the system. Significantly, it is demonstrated that the energy-momentum tensor of the effective matter distribution plays a crucial role in the considered system.

In summary, this abstract provides a comprehensive overview of different cosmological models, highlighting the shift from Newton's static universe to the expanding universe described by Friedmann equations. Additionally, it presents an original approach to understanding charged ultra-dense strange quark stars within the framework of modified  $f(R, T)$  gravity theory. The implications and significance of this research lie in uncovering the effects of modified gravity on the structure of these exotic celestial objects.



## Monte-Carlo simulation to study a liquid like system

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Monte-Carlo method has been powerful tool in the field of simulation since its inception. Our work is based on studying a system of particles using Monte Carlo simulation with control parameters, temperature and number density, taken in the liquid regime. For this study, we calculated two correlation functions –  $Q(t)$  (time correlation function, that gives us information about dynamics) and  $g(r)$  (the pair distribution function, that gives us information about structure).  $Q(t)$  quantifies the correlation between two configurations separated by time,  $t$ ,  $g(r)$  gives us information about the structure of the system. The variation of  $g(r)$  with temperature and number density has been reported.



## Hydrofuel – A future source of energy

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Hydrofuel is expected to be widely used in the near future as most of the other energy resources are non-renewable and possess huge environmental risks. Like all other energy sources, hydrofuel has merits and demerits too. Here, in our presentation, we have tried to find the ways by which we can prevent the challenges of using this energy resource.



## Distinction Between Classical Point of View & Quantum Point of View

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Our motive behind the poster presentation is to represent the visualization of the difference between classical and quantum mechanical approach of observation. Here in this pictorial presentation, we tried to show some examples to distinguish between the two with very basics of nature's philosophy. We tried to highlight some very basic points and equations in our presentation. We have tried to discuss concepts of discreteness of energy, wave-particle duality, Schrodinger wave equation, Born's probabilistic interpretation, Heisenberg's Uncertainty Principle etc



## Solving Bernoulli's Equation by Variable Separation

Upamanyu Ghose

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Differential Equations have a wide range of applications in Physics, both Ordinary and Partial. Mathematical Modelling is an important aspect of application of Differential Equations. Ordinary differential equations are of 2 types, 1) Linear 2) Non linear. I have decided to explore the non linear branch of ODEs ,especially Bernoulli's Equation ( $y' + p(x)y = q(x)y^n$ ,  $n \neq 0, 1$ ), and present a poster on this topic. The conventional method of solving Bernoulli's Equation utilises the concept of transforming the non linear ODE into a linear ODE by making a substitution and solving the corresponding linear ODE to get a desired solution. However, I have attempted to solve Bernoulli's Equation by Variable Separation Technique, the easiest approach to solve a differential equation and is very handy , and I also got the desired results as well. Thus, I intend to explore this particular non linear ODE by the use of Variable Separation Technique and may conclude that many ODEs can be solved by Variable separation instead of Linear Transformation. This may open a new avenue for many researchers who would like to work on Mathematical Physics or the ones who would encounter Non Linear ODEs during any process and be able to solve them by this technique in a few steps.

Moreover, I intend to use an example of a Bernoulli's Equation that can be solved by using inbuilt Python libraries such as Scipy,Numpy and Matplotlib ,solve it by computational techniques in Python, plot the solution curve and present it along with the code on the poster.This will ensure that the Bernoulli's Equation can be solved by using Computational technique and can be verified with the analytical solution obtained by Variable Separation, thus to validate my approach. This entire poster will help many future research scholars like me to develop a new understanding non linear ODEs and may contribute towards the working out of the solutions of several non linear ODEs which are yet to be solved, and are intriguing research problems.

## Bound and Resonance $^3F^e$ States of Helium Atom under Plasma Confinement

<sup>1</sup>A. N. Sil, <sup>2</sup>S. Dutta, <sup>3</sup>D. Ghosh, <sup>4</sup>J. K. Saha, <sup>2</sup>S. Bhattacharyya and <sup>5</sup>Tapan Kumar Mukherjee

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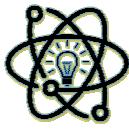
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The studies on the structural and spectral properties of Helium or Helium like systems have got especial attention in the scientific community since the birth of quantum mechanics due to the non-separability of the dynamical equation of motion of three body systems. It provides a fundamental testing ground to verify the accuracy of different quantum mechanical approximation methods. Researchers have examined atomic systems in different mediumenvironments during the last several decades because they provide useful information about the environment. Among those external environment atomic structure calculations, plasma medium is of particular interest as they reveal a wealth of important information on the diagnostic determination of the plasma. For Helium like systems, doubly excited states (DESs) play an important role in the plasma diagnostic purpose [1]. It is to be mentioned that almost all the works are restricted up to L=2 angular momentum states (D-state) [1]. Few works can be found [2-3] that deal with the F-states (L=3) under a plasma medium.

Under such circumstances, we have performed calculations for meta-stable bound and resonance  $^3F^e$  states of helium atom under a weakly coupled plasma environment where it is assumed that all the particles within the atom interact via exponentially screened Coulomb potential. Variation method is employed by using multi-exponent Hylleraas basis sets [4] to ensure the explicit inclusion of electron correlation effects. The basis set contains total of 900-terms and the energy eigenvalues of the metastable bound  $^1,3F^e$  states are obtained in the framework of Ritz variational principle. Resonance parameters (energies and widths) for a wide range of resonance states ( $^{1,3}F^e$ ) of helium below  $N = 3$  and  $N = 4$  ionization threshold of  $\text{He}^+$  have also been evaluated by using the stabilization method [5]. MBS energies show good agreement with those available in the literature [2-3]. The present resonance parameters below  $N = 3$  ionization threshold of  $\text{He}^+$  are in excellent agreement with the available accurate theoretical results [2]. For the first time, we have found the resonance states ( $^{1,3}F^e$ ) of helium atom above  $N = 3$  ionization threshold of  $\text{He}^+$  under a plasma environment. Variation of other structural properties such as one- and two-particle moments, inter-electronic angles etc., of  $^{1,3}F^e$  states of Helium atom are estimated for the first time in the literature with respect to different screening parameters



of the exponentially screened Coulomb potential. To interpret complex atomic spectra obtained in laboratory plasma experiments and in astrophysical observations, such theoretical investigations are necessary. The present method can be applied for other resonances of different symmetries with a sufficient number of terms in the Hylleraas basis set to yield accurate structural information of Helium-like systems.

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## Dielectric Properties of ZnTe Nanomaterial

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In recent times, nanomaterials and semiconductors have emerged as crucial components, offering the ability to manipulate their properties according to specific requirements. This study focuses on the synthesis of type II-VI semiconductor ZnTe nanomaterials via a soft chemical route, as discussed in Section 2. Subsequently, Sections 2 and 3 develop into the analysis of the material's structure through X-ray diffraction and transmission electron microscopy techniques. The investigation also includes frequency and temperature-dependent experiments to unravel the dielectric properties of ZnTe nanomaterials. These findings are also presented in Sections 2 and 3.

Section 4 presents the conclusions drawn from the experimental results, highlighting the dependencies of various properties such as impedance, dielectric constant, electric modulus, and dielectric loss. The graphical representations of these properties were obtained through experimental data collection. The first Section provides a theoretical overview of semiconductors, nanoparticles, and the dielectric properties of matter, setting the foundation for the subsequent Sections.

Overall, this study contributes to the understanding of ZnTe nanomaterials, their structural characteristics, and dielectric properties. The synthesized materials hold potential for various applications, particularly in the field of advanced electronics and optoelectronic devices.

## A brief review on smart materials

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Many electroactive functional materials have been used in small- and microscale transducers and precision mechatronic control systems for years. However in the mid-1980s scientists started integrating electroactive materials with large-scale structures as in situ sensors and actuators, thereby introducing the concept of smart materials, smart structures, and structronic systems predominantly to the society. Smart materials are a family of materials, listed in advanced materials, having a structure at the nano-structure level that responds in a controlled and particular way to different types of influences (to which a particular material is sensitive) upon it. These groups of materials have self-accommodation with environment and they are classified according to their responses, such as physical (pressure, temperature, humidity, light, electric field, magnetic field, etc.), chemical (pH, CO<sub>2</sub>, etc.), or biological (enzymes, hormones, etc.) stimuli. Smart materials are getting high attentions due to their commercial applications such as actuator or sensor, self-healing materials, medical instruments and machineries and so on. This dissertation work demonstrates a brief review on different types of smart materials with their specific characteristics, limitations and applications along with their current status. Also we shall discuss here about the current experimental status as well as the improvements of the smart material properties can be made. Also an over view on the fertile potential research areas and future applications shall be discussed in this project work.



## Recent Advancements in Blood Glucose Monitoring Technology

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Determination of approximate concentration of glucose in blood is a common medical investigation. For the past few decades the technology for blood glucose monitoring, essential for diabetes management, has been evolved greatly to get ideal and reliable results. While device like Glucometer measure glucose levels at a single moment of time, Continuous Glucose Meter (CGM) system continuously check glucose level throughout day and night and is thus very much beneficial for diabetes self-management. Blood Glucose monitoring system works through an electrochemical biosensor ( basically a transducer). Since its introduction in 2000, CGM has become one of the mainstream technology in blood glucose monitoring and is expected to grow even faster for the technological advancement. Now a days CGM can be connected to smart phones and the CGM sends data to the smart phone via Bluetooth. Optical sensing technology provides an interesting alternative to more established electrochemical sensors and contributes to better flexibility concerning the design of CGM system , their cost, material used etc. With time the device is getting smaller, more comfortable to wear, accurate and even non-invasive. Patch pump, glucose sensing lens are some trending technologies of future. Technological advances including CGM, connected insulin pens, insulin pumps and automated insulin delivery algorithm, in an integrated way is making it possible to achieve the optimal control of diabetes for the insulin users.

# Layer- by- layer electrostatic self assembled film of anionic dye sulforhodamine B and a cationic bio polymer Poly-L-Lysin: A spectroscopic and Atomic force microscopy study

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One of the most rapidly growing means of preparing thin films for materials science research is the layer-by-layer (LbL) self-assembly method which utilizes the alternate adsorption of oppositely charged molecular species onto solid substrate via electrostatic interaction. This method becomes popular because of its nanoscale control over the molecular architectures, ease of film fabrication, less experimental sophistication etc. In recent time low molecular weight water soluble fluorescent organic materials attracted significant attraction because of their implication in numerous fields such as biomedicine and drug delivery, optics, sensors etc. In this poster presentation we report the photophysical and spectroscopic study of negatively charged small molecule organic dye Sulforhodamine B(SRB) and positively charged biopolymer Poly- L-Lysin(PLL) organized in Layer by Layer self assembly film onto a solid substrate.Uv-Vis absorption and fluorescent studies have been carried out to understand nature of binding between SRB and PLL on solid substrate. Absorption and fluorescent studies has also helped us to understand aggregation phenomenon of SRB molecules in restricted environment of LbL film. As PLL undergoes structural changes in response to a change in pH of the solution, the adsorption of SRB on the backbone of PLL is strongly dependent on solution pH. Atomic force microscopy images on LbL film revealed the surface morphology and roughness profile of SRB-PLL molecular assembly on solid substrate.



# Magnetosonic Shocks and Solitons in Fermi Plasma with Quasiperiodic Perturbation

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In this paper, we consider dense stellar plasma consisting of predominantly electrons, positrons, and ions under the action of the magnetic field of the star. We derived the KDV-Burgers equations by using the reductive perturbation technique and obtained shock and solitary profiles for magnetoacoustic waves. We further studied the self-interaction of such stationary formations and the amplitude-modulated envelope solitons. The possibility of a rogue wave-like structure is also discussed. To understand the physical problem in greater detail, we studied the Hamiltonian formulation to study the stability. We studied how modulational instability can lead to the formation of rogue waves by investigating the non-linear Schrodinger equation. Additionally, drift-like instability showing the density and charge separation effects in plasma has been studied. The results will be helpful to interpret magnetoacoustic wave formations in solar corona or other stellar entities and can help in the study of inhomogeneous plasmas in laboratory and fusion reactors.

## Characteristics of isotherm and Schottky diode of lead (II) iodide coordinated azo-imidazole by Langmuir-Blodgett technique

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Functional organic materials, in recent years, with dense  $\pi$ -conjugated electron clouds have drawn immense attention for development of various electronic and optoelectronic devices. Imidazole derivatives, among different organic materials, are promising for their unique electronic structures which result tunable electric and/or optical properties. Imidazole containing azo dye is potential for dye sensitized solar cells (DSSC), photo-switchable inhibitors, molecular switching, anti-mycobacterial activity etc. Again, for fabrication of nano-dimensional thin film, Langmuir-Blodgett (LB) technique is most unique and best technique to construct uniform 2-dimensional device. This gives molecular level control over film thickness with highly ordered nanostructures.

In this work, we organize and develop (azo)-imidazole derivative namely lead (II) iodide Complex of 1-alkyl-2-(arylazo) Imidazole onto solid substrates and characterize its optical and electrical properties. The compound, having hydrophilic imidazole ligand and long hydrophobic alkyl chain, is a LB compatible material. Surface pressure-area ( $\pi$ -A) isotherm study shows uniform monolayer formation at air-water interface. Association and phase behaviour are studied by compressibility analysis. Brewster angle microscopic (BAM) images at different surface pressure shows successful molecular aggregation at air-water interface. UV-vis absorption spectroscopic study of LB film shows slight red shift of absorption spectra as compared to pure compound/chloroform solution which reveals J-aggregation on solid support. Organization of film indicates dense accumulation of molecules by increasing surface pressure. Layer variation of LB film shows gradual increase of absorption spectra which is the indication of high degree of deposition, film homogeneity and reproducibility. Current-voltage characteristics is measured by constructing Au/LB film/ITO Schottky junction which reveals potential applicability of the compound towards future organic electronic devices.

## Fabrication of multifunctional PVDF/rGo Composites and their enhanced dielectric properties.

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A new two-step process was developed to prepare PVDF/ reduced graphene oxide (PVDF /rGO) Composite films: the synthesis of PVDF/GO Composite film and immersion of such films in hydrobromic acids for reduction. rgo /PVDF Composites with excellent absorption properties were obtained and characterized. Reduced graphene oxide Composed of reduced graphite oxide have been fabricated by an in situ growth method under mild wet chemical Conditions(140°C). The rGO effect on electrical Conductivity was measured and the result indicated an increasing in electrical Conductivity by increasing the graphene content. The enhanced absorption and dielectric properties were investigated; the results indicated that for the composites with a low filler loading of 0.1 wt%, the maximum reflection loss of the PVDF/ RGO Composites can reach 10 for 100 to 80 at 1 KHZ. The fabrication and evolution of a high performance piezoelectric and ferroelectric material based poly(vinylidene fluoride) - reduced graphene oxide barium titanate (PVDF - RGO-BTO) ( $\text{BaTiO}_3$ ) nanocomposites have been investigated. As a result, the improved piezoelectric and ferroelectric properties made the PVDF/rGO Composites film with 0.1 wt% RGO content much better piezoelectric energy transfer and ferroelectric Storage in materials than the neat PVDF which may be employed in electronic industry for development of next generation flexible energy Storage devices. Fabrication rGO / PVDF membranes were achieved to the enhanced performance of the system.



## Preparation of PVDF/GO nanocomposite films exhibiting largely enhanced dielectric properties

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In recent years, there is an increasing interest in the flexible polymer nanocomposites with dielectric constant because they possess exceptional electrical, mechanical and optoelectronic properties. In this work, PVDF/GO nanocomposite films were prepared by simple solution casting method. Different weight percentage of GO, ranging from 1wt% to 10wt%, were dispersed in the PVDF solution. The structural and morphological characterizations of PVDF/GO nanocomposite films were carried out using techniques such as X-ray diffraction (XRD) and Scanning Electron Microscopy (SEM). The XRD analysis confirmed the presence of GO in the nanocomposite films, and SEM images revealed a homogeneous dispersion of GO within the PVDF matrix. The dielectric properties of the PVDF/GO nanocomposite films were evaluated using LCR meter. The results showed a significant enhancement in the dielectric constant and AC conductivity of the composite films with increasing GO content. The PVDF/GO nanocomposite films exhibits good mechanical flexibility and thermal stability, making them suitable for various applications in electronic devices and energy storage system.

# Influence of water sorption on ionic conduction of polymer composite film

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Polymer matrix/composite has been identified and applied by researchers owing to its numerous advantages over Glass, alloys etc. In this context, Poly (ethylene) oxide is widely used in various field in application like solid polymer electrolyte, controlled drug delivery system, fuel cell, sensor etc [1,2]. Therefore, the properties of the polymer composites should be tailored based on the specific applications. The primary restriction of a polymer system is its lower conductivity. Owing to this aspect, polymer – ion (i.e salt) composite is one of the most availed research for wide application. In this context, hydrogen ion transport / conduction forms the basis of ionic conduction for a number of composites. In this aspect Saha et al have reported the detailed study on the synthesis and characterization of Poly(ethylene oxide) composites synthesized with salts like NH<sub>4</sub>I and KBr [3,4]. The study reflects the increase in conductivity of such by many orders compared to pristine polymer system. The respective FTIR analyses also support the bond formation in the formed composite along with the extent of free and bonded ions. Water sorption and ion diffusion can significantly alter the chemical and mechanical properties of polymeric-based components over time. The sorption mechanisms for water uptake can be attributed to chemical and morphological properties of materials. The primary objective of this research is to determine the diffusion coefficient of polymer salt composite by the soaked and re dying process of the system. Finally, the diffusion mechanism of the hydrated polymer films is analysed theoretically. This suggests the presence of two types of water within the polymer matrix; a less mobile phase of absorbed water that is interacting strongly with the polymer matrix and a more mobile phase of absorbed water residing within the cracks and a more mobile phase of absorbed water residing within the cracks.

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## s-, p- & d- wave phase shifts in Ps – He scattering using a Static Exchange Model

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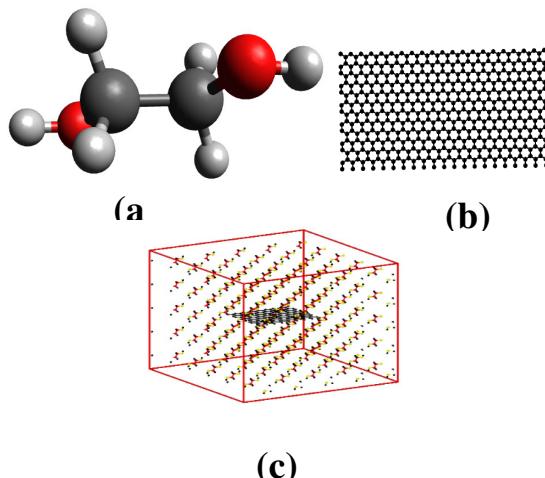
Scattering of Positronium atom (Ps) off the He atom has been investigated theoretically at low energy using Static Exchange Model. Hylleraas and Hartree- Fock wave functions for He atom are used in the calculation. The s- , p- and d- wave phase shifts along with total elastic cross-sections are reported and compared with the available results of others. The effect of electron exchange between the projectile and the target atoms is found to be significant in the low energy range.

# Viscosity of Ethylene Glycol (EG) base fluids containing Graphene Nanosheets (GNS): Insight from Molecular Dynamics

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To determine the viscosity of ethylene glycol (EG) base fluids including graphene nanosheets (GNS), the EMD simulation is used within the Green-Kubo framework. The effects of temperature (285 K - 313 K) and GNS-1, GNS-2, and GNS-3 on viscosity have been investigated. Both the base fluids and nanofluids have a viscosity that decreases with temperature. The radial distribution function (RDF) of nanofluids has been studied.



**Figure** (a) Geometrical structure of ethylene glycol.(b)Geometrical structure of graphenenanosheet. (c)Snapshot of the initial molecular dynamics model using OVITO for 140 pure ethylene glycol and graphene nanosheets.

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# Crystal Structure of 3-phenylsulfoxyl coumarin derivatives

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## 1. Introduction

Coumarin derivatives have different biological activities including spasmolytic, antiarrhythmic, cardiotonic and antitumor properties. Some of the coumarin derivatives have weak estrogenic activity, so they were used as therapeutic agents to prevent menopause related diseases. Besides these, coumarin derivatives have also been used in solid photochemical reactions and dye- laser studies.

So, it is important to make a systematic structural and interaction studies of these types of coumarin derivatives(including 3 – phenyl sulphonyl coumarin) in their crystals. These results of structural, packing and noncovalent molecular interaction (such as H-bonds, aromatic  $\pi$  -  $\pi$  interaction in the crystal may help to design the more potent bio-active compounds with unique feature and activity. We have analyzed the structure of 3 -phenyl sulphonyl coumarin by x-ray crystallography methods and also analyzed the conformational and electronic consequences of this compound by DFT - methods and Hirshfield calculation.

## 2. Material and Methods

### 2.1. *X-ray Crystallography studies:*

X raydiffraction data for the crystalline compound of chemical formula  $C_{15}H_{10}SO_3$  were collected at temperature of 114K on a diffractometer equipment with Bruker Kappa Apex -II CCD area detector using  $CuK\alpha$  ( $1.54178\text{\AA}$ ) X -ray source. The structure was solved by direct method and refined with a full-matrix least squares refinement (total number of refined reflections 2098) using SHELXL-2017 program [4] with R value 0.056.

### 2.2. *Computational Studies:*

The structure of 3-phenylsulfoxyl coumarin was build and optimized (steepest descent method) with CHARMM forcefield until the structure reached a convergence gradient of 0.001kcal/mole using Hyperchem 7.2 program[1]. The molecule was further optimized with B3LYP/def2-svp level of theory using orca 5.0.1 computational program[2]. Absence of any negative frequency at same

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level of theory confirmed the global optimization of the compound. The Hirshfeld calculations are done using Crystal Explorer computational program[3].

### 3. Results and Discussion

The structure of 3-phenylsulfoxoy coumarin (Figure 1a) was optimized (Figure 1b) and different electronic properties were studied like HOMO, LUMO,  $\Delta E$ , Hirshfield calculations (Figure 2 and 3). The HOMO, LUMO and  $\Delta E$  are observed to be -6.3846, -2.3129 and 4.0717 eV respectively.

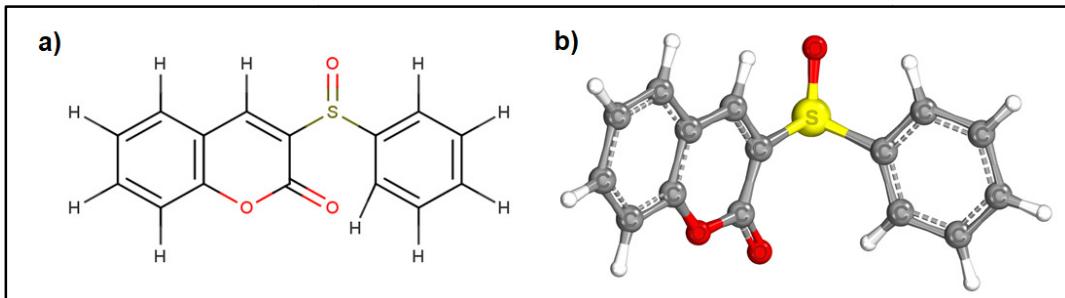


Figure 1. Structure of 3-phenylsulfoxoy coumarin. a) 2D structure b) 3D DFT optimized structure

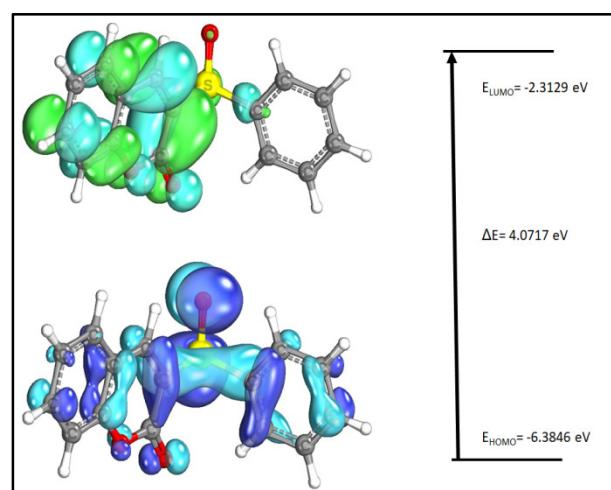


Figure 2. HOMO, LUMO and  $\Delta E$  for  
3-phenylsulfoxoy coumarin

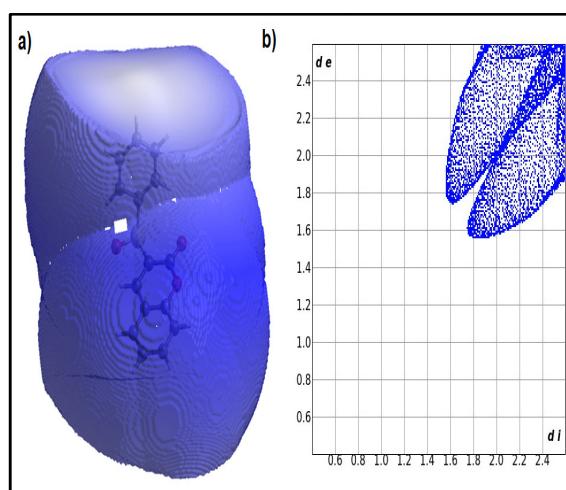


Figure 3. Hirshfeld calculation

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## Theoretical study on structure, dissociation pathways and thermochemical analysis of R-CN (R= CH<sub>3</sub>-, CH<sub>2</sub>CH-, CH<sub>3</sub>CH<sub>2</sub>-) molecules.

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The field of astrochemistry and astrobiology has gained immense attention to the scientists due to the recent development in high precession telescope used in space mission to study the composition of different interstellar media and planetary atmosphere. Out of the recent detections, Voyager-II found the existence of CH<sub>3</sub>CN, CH<sub>2</sub>CHCN and CH<sub>3</sub>CH<sub>2</sub>CN in the surface of Titan (Saturn's largest moon). The presence of -CN fragment in the molecule makes these molecules possible precursor amino acids and finally biological molecules, hence these are often considered as a prebiotic substance towards the origin of life. The detailed mechanism of the dissociation and reaction pathways is still a challenging to the researchers. In this work we have adopted theoretical approached both ab-initio and DFT method to study their structure, properties and possible reaction channels. Very popular and widely used hybrid functional B3LYP method is used for optimization followed single point energy calculation by QCISD and CCSD(T) methods. The reported structural parameters, vibrational frequencies and dipole moments yield good agreement with available reported experimental results. We reported four dissociation channels of CH<sub>3</sub>NC and five channels of CH<sub>2</sub>CHNC and CH<sub>3</sub>CH<sub>2</sub>NC. Out of all these dissociation channels the most favourable channel consists of HCN product having dissociation energy of ~16 kcal/mol and 6-7 kcal/mol for CH<sub>2</sub>CHNC and CH<sub>3</sub>CH<sub>2</sub>NC molecules respectively.

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## Evaluation of the activation energy of thermal peaks recorded under quadratic heating scheme without prior knowledge of order of kinetics

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In the present article we have developed a method of determination of the activation energy of thermoluminescence (*TL*) peaks recorded under quadratic heating scheme. Usual methods of determination of activation energy of *TL* peaks require the prior knowledge of order of kinetics. But the determination of order of kinetics is not straight forward. In view of this we have proposed a method of determination of the activation energy of a *TL* peak recorded under quadratic heating scheme. The method does not require the prior knowledge of order of kinetics. The method can also be extended to determine two other trapping parameters namely order of kinetics and frequency factor. The suitability of the present method has been assessed by applying it both to numerically computed and experimental results of *TL* peaks.

## Analyzing the Generalized Coherent States for Free Particles

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Free particle in quantum mechanics is a very important topic. But the coherent state analysis hasn't been untouched for long. Recently it has been studied in the semi classical domain. Lately a free particle solution was described using the linear non-Hermitian invariant operator. In this work we will study the Schrodinger equation which can be derived using a simpler method based on a Hermitian linear invariant operator and exact Gaussian wave function that corresponds to a coherent state solution will be obtained from this method and explanation for the general Quantum provided in the Lewis-Risnfield framework is now re-examined for a Quantum classical system.

## Synthesis of Ni(OH)<sub>2</sub>nano powder by electrolyzing mechanism and investigation ofphotocatalytic and supercapacitorproperties

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Nickel hydroxide nanopowder has been synthesized by a unique electrolyzed mechanism where the electrolyte is not a salt solution of electrolyzing material but a pure NaCl solution. The electrolyzing material (Ni) has been used as an anode, and a copper plate as the cathode with a 5V potential difference between the two electrodes. Unlike the formal electrolyze, no nickel reached the cathode side,whereas they combined with OH<sup>-</sup> on electrolyte solution. The photocatalytic property is investigated by Rhodamin B (RhB) dye degradation using a 500W halogen lamp. Two dissimilar metal pieces were used to investigate the electrolytic property of the synthesized nickel hydroxide and it behaves as a good inorganic solid electrolyte.



## *Invited Scientific Articles*

# MEDICAL PHYSICS – Application of Physics in Medicine

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Ph.D., Post. M.Sc. Dip.R.P, R.S.O, M.Sc.(Physics)

**Medical Physics** Deals with the application of the principles and methods of Physics in diagnosis, treatment and prevention of human diseases. Medical Physicists are mainly health care professionals with special education and training in the concepts and techniques of applying Physics in medicine.

They are traditionally found in the following healthcare specialties:

**A) Radiotherapy or Radiation Oncology** which is mostly used modality of treatment for cancer patients. In this modality, very high energy X-ray or gamma ray and also particle radiation like electron beam, proton beam, neutron beam,  $\alpha$  particle, heavy ions are used to kill cancer cells to control cancer or to destroy those cells completely to cure cancer. In this specialty, Medical Physicists deals with radiation generating equipment like Mega-Voltage X-ray emitting machines such as Linear Accelerator, Tomotherapy, Cyber-knife and High Energy Cyclotron for producing charged particles and internal and very conformal radiotherapy machine like Brachytherapy machine. In recent advancement, very sophisticated proton beam, neutron beam,  $\alpha$  particle and heavy ion beam therapy are being practiced in developed countries for treatment of cancer. One proton beam therapy machine also has been functioning in India. Under department of Atomic Energy, one more proton therapy machine is going to be commissioned in Mumbai very shortly in Tata Memorial Hospital.

Medical Physicists bring a unique perspective to the clinical team in a radiation oncology department: that of a scientist trained in Physics, including Radiological Physics, and also in clinical and basic medical sciences as well as radiological sciences. The medical physicists perform an important role working along with radiation oncologists, radiotherapy technologists and others to assure accurate delivery of all aspects of a radiation treatment prescription. Medical physicists are also responsible for the precision and accuracy of treatments by using advance software to develop an individual patient treatment plan. They are responsible for supervising the correct functioning of the equipment producing ionizing radiation as well as all dosimetry and other auxiliary equipment.

Other responsibilities of medical physicists in a radiotherapy department:

- 1) Planning for radiation therapy departments, radiation shielding calculations as per guidelines from competent authority and proper designing of the bunker where radiation equipment to be installed.

- 2) Equipment usage, selection and replacement.
- 3) Supervise installation of radiation equipment.
- 4) Quality control check and all acceptance tests for newly installed radiation machine as per guidelines published by competent authority and commissioning of new equipment.
- 5) Calibration of all radiation sources used in the department.
- 6) Development and maintenance of a quality assurance program for all radiation equipment as well as dosimetry equipment.
- 7) Development and administration of the radiation safety program including compliance with all regulating and certifying agencies.
- 8) Design and fabrication of treatment aids and treatment beam modifiers.
- 9) Development of the techniques (hardware, software and procedural) to improve the quality of delivery of radiation treatment.
- 10) Teaching medical physics and radiation safety as per curriculum for post graduate medical students, Post M.Sc. Medical Physics students and radiation technologist students.
- 11) Continuing periodic education program in routine use and handling of radiation equipment and radiation safety program for radiation oncology staffs.
- 12) Administration of radiation personnel monitoring program for all radiation workers in the department. Radiation safety aspects of general public is other important issue to look after.
- 13) Participation on the Institutional Radiation Safety Committee and other safety committee to prepare guidelines for the Institute as per recommendations of the competent authority.

**B) Nuclear Medicine:** It is a medical specialty involving application of radioactive substances in the diagnosis and treatment of diseases. Nuclear medicine imaging in a sense is “Radiology done inside out” because it records radiation emitting from within the body rather than radiation that is generated by external sources like X-ray. In addition, Nuclear medicine scan differ from radiology as the emphasis is not on imaging anatomy, but on the physiological functional status of the organ. For such reason it is called a physiological imaging modality. Single photon emission computed tomography (**SPECT**), and Positron emission tomography (**PET**) are two most common imaging modalities in nuclear medicine.

In nuclear medicine imaging, radioisotopes are tagged with organ specific radiopharmaceuticals are taken internally through intravenous injection, orally or through inhalation. After specified time, patients are positioned under **SPECT or PET**, the external radiation detectors capture gamma

radiation emitted from organs where radiopharmaceuticals are deposited. Finally, collected data after processing produces three dimension images with the help of image processing algorithm and processing software.

### **Reactor and Medical Cyclotron:**

In SPECT, reactor produced radio-isotopes like Mo<sup>99m</sup>, I<sup>131</sup> etc. are used. In generator system, Tc<sup>99m</sup> are extracted from Mo<sup>99m</sup> in Nuclear Medicine Laboratory and tagged with organ specific radiopharmaceuticals to diagnose different diseases. In India, we have number of such reactors in Bhabha Atomic Research Centre, Mumbai. All Nuclear Medicine Laboratories usually procure such isotopes from B.A.R.C.

Positron emitting radio-isotopes are used in PET scanning. Positron emitters are produced in Cyclotron. F<sup>18</sup>, O<sup>15</sup>, N<sup>13</sup>, C<sup>11</sup> are very useful isotopes for PET scanning. Except F<sup>18</sup> rest of the isotopes are very short lived. In house Medical Cyclotron is essentially required for use of O<sup>15</sup>, N<sup>13</sup>, C<sup>11</sup>. In Kolkata, one Cyclotron commissioned in New Town by Siemens to produce F<sup>18</sup> (Half-life- 109.8 min). Seven PET scanning Centre in Kolkata procure F<sup>18</sup> from there.

### **Role of clinical medical physicist in Nuclear Medicine:**

The clinical medical physicist qualified in Nuclear Medicine imaging brings a unique perspective to the clinical team in nuclear medicine imaging department: A scientist trained in physics, including imaging and radiological physics and also basic medical, clinical and radiological sciences.

### **Responsibilities of a clinical medical physicist in Nuclear Medicine:**

- 1) Specification of new equipment
- 2) Supervision of acceptance testing and performance verification of all imaging equipment.
- 3) Supervision of calibration, preventive maintenance, repair of equipment and documentation of all relevant information.
- 4) Development and maintenance of a quality management program for all imaging equipment to facilitate the production of images of optimum quality while minimizing radiation doses to the patient.
- 5) Responsibilities of all instrumentations required for quality control and image quality and patient exposure measurement.
- 6) Determination of doses from radiological procedures.
- 7) Establishing and maintaining a good radiation safety program.
- 8) Supervision of the preparation, handling and disposal of radionuclides.



- 9) Participation in the institutional radiation safety committee and other relevant committee.
- 10) Determination of shielding required for new or renovated equipment rooms for ionizing radiation.
- 11) Design of special shielding devices.
- 12) Facilitation of compliance with all regulating and certifying agencies.

**Minimum qualification for Medical Physics Practice in India:**

- 1) Post Graduate Degree in Physics
- 2) Post M.Sc. Diploma in Radiological/Medical Physics from recognized Universities.
- 3) An internship of 12 months in a well-equipped radiotherapy department.

**OR**

- 1) A basic Degree in Science with Physics as Major subject.
- 2) A Post Graduate Degree in Radiological or Medical Physics from a recognized University.
- 3) An internship of 12 months in a well-equipped radiotherapy department.

**List of Medical Physics courses in India:**

- 1) Radiological Physics and Advisory Division, Bhabha Atomic Research Center, Mumbai.
- 2) Anna University, Chennai
- 3) Jadavpur University, Kolkata
- 4) IIT Kharagpur
- 5) NISER, Bhubaneswar,
- 6) IIT Hyderabad and some other

**Nuclear Medicine Technology course in India:**

Minimum eligibility criteria for enrolling in this courses are Graduate with Physics as major subject.

- 1) Radiation Medicine Center, Bhabha Atomic Research Center, Mumbai.
- 2) Tata Memorial Hospital, Mumbai.
- 3) JIPMER, Puducherry.
- 4) AIIMS, New Delhi.
- 5) SGPGIMS, Lucknow.

# What are nanomaterials, and how do we characterize them?

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## What does nano mean?

The term "nano" is a prefix derived from the Greek word "nanos," which means "dwarf." In the context of measurements and scale, "nano" is used as a metric prefix denoting one billionth (1/1,000,000,000) of a unit. It is symbolized by the prefix "n." It can indicate length as a nanometer (nm), time as a nanosecond (ns), or weight as a nanogram (ng) etc. As we do not deal with such numbers, it is tough to comprehend any number that is just a fraction of a billion. The following provides a few examples to comprehend such a small number.

1. On average, human hair has a diameter of about 80,000 to 100,000 nm. This means that a nanometer is about 100,000 times smaller than the diameter of a human hair.
2. Virus Size: Some viruses, such as the influenza virus, have a size range of about 80 to 120 nanometers. So, a nanometer is roughly the size of a single particle of a small virus.
3. DNA Double Helix: The diameter of a DNA double helix is approximately 2 nanometers. This means that if you were to stretch out the width of a DNA molecule, it would be just a few nanometers wide.
4. Transistors: In modern computer processors, the size of individual transistors is often measured in nanometers. For example, a 14-nanometer transistor technology means that the smallest feature on the chip is about 14 nanometers wide. This miniaturization allows more transistors to be packed onto a single chip, increasing their processing power.
5. Atoms and Molecules: The size of atoms and molecules typically ranges from a fraction of a nanometer to a few nanometers. For instance, a water molecule has a diameter of about 0.3 nanometers, while a carbon atom has a diameter of around 0.15 nanometers.
6. Light travels approximately 30 centimeters (about 1 foot) in one nanosecond.

These comparisons provide a sense of scale for understanding the tiny dimensions associated with nanometers. The nanoscale is where many fascinating phenomena occur, and nanotechnology enables us to manipulate and explore this realm for various scientific and technological advancements. Often the properties of bulk systems change when they are made to nanoscale dimensions.

### How do the properties of a metal change when it is made to a nanoscale dimension?

The properties of metals can undergo significant changes when transitioning from the bulk scale (macroscopic level) to the nanoscale (nanoscale level). Some of the notable changes include:

1. Melting Point and Boiling Point: The melting and boiling points of metals may decrease as their size is reduced to the nanoscale. This occurs due to the increased surface area-to-volume ratio, which leads to enhanced surface effects and weaker interatomic bonding.
2. Mechanical Properties: At the nanoscale, metals often exhibit improved mechanical properties, such as increased hardness and strength. This phenomenon, known as the "smaller is stronger" effect or the Hall-Petch effect, arises due to grain boundary strengthening. The presence of a larger number of grain boundaries in nanocrystalline metals restricts the motion of dislocations, resulting in enhanced mechanical properties.
3. Electrical Conductivity: Metals are known for their excellent electrical conductivity at the bulk scale. When metals are reduced to the nanoscale, their electrical conductivity can be influenced by quantum confinement effects. As the size of metal particles decreases, the scattering of electrons at the boundaries becomes more significant, leading to changes in electrical conductivity.
4. Optical Properties: Metal nanoparticles exhibit unique optical properties due to the phenomenon called localized surface plasmon resonance (LSPR). LSPR occurs when the collective oscillations of free electrons on the nanoparticle surface interact with light, leading to enhanced absorption and scattering of specific wavelengths. This property is extensively utilized in various applications such as sensing, imaging, and nanophotonics.
5. Surface Reactivity: Metal nanoparticles have a significantly higher surface-to-volume ratio compared to bulk metals. This increased surface area can result in enhanced surface reactivity, making the nanoparticles more reactive and susceptible to chemical interactions. This property is exploited in catalysis, where metal nanoparticles act as highly efficient catalysts due to their increased surface activity.

It is important to note that the specific changes in metal properties from bulk to nanoscale can vary depending on factors such as the metal type, size, shape, and fabrication methods. Nonetheless, these general trends provide an understanding of how metal properties can be altered when working at the nanoscale.

### How do the properties of a semiconductor change when it is made to a nanoscale dimension?

Similarly, the properties of semiconductors can undergo significant changes when transitioning from the bulk scale (macroscopic level) to the nanoscale (nanoscale level).

1. Bandgap Engineering: Semiconductors have a characteristic energy bandgap that determines their electrical conductivity. When semiconductors are reduced to the nanoscale, the quantum confinement effect comes into play. As the size of the semiconductor nanostructures decreases, the electronic energy levels become quantized, resulting in a widening of the bandgap. This phenomenon is known as "bandgap engineering." By controlling the size and shape of semiconductor nanoparticles, their bandgap can be tuned, leading to modified optoelectronic properties.
2. Quantum Confinement Effects: In nanostructured semiconductors, such as quantum dots (we discussed more in a later section) and nanowires, the confinement of charge carriers in all three dimensions leads to quantum confinement effects. This confinement alters the energy levels, density of states, and electronic behavior of the semiconductor. The discrete energy levels available to electrons and holes in nanostructures result in unique electronic and optical properties.
3. Enhanced Optical Properties: Semiconductor nanoparticles at the nanoscale exhibit size-dependent optical properties. This includes the phenomenon of quantum confinement, where the energy of absorbed or emitted photons is related to the size of the nanoparticles. As the size decreases, the bandgap energy increases, resulting in a blue shift in the absorption and emission spectra. This property is utilized in various applications such as quantum dots for displays, light-emitting diodes (LEDs), and photovoltaics.
4. Surface Effects: Semiconductor nanostructures have a large surface-to-volume ratio compared to bulk materials. This increased surface area can lead to enhanced surface effects, such as increased surface reactivity and sensitivity to environmental conditions. Surface states and surface passivation play a crucial role in the electrical and chemical behavior of semiconductor nanostructures.
5. Charge Carrier Mobility: The charge carrier mobility, which determines the ease of charge transport, can be influenced by defects and impurities in semiconductors. In nanostructured semiconductors, the presence of a high density of interfaces and surfaces can affect the charge carrier mobility. The scattering of charge carriers at interfaces and surfaces can result in reduced mobility compared to bulk semiconductors.

These changes in semiconductor properties at the nanoscale have significant implications for various applications, including nanoelectronics, optoelectronics, sensors, and energy devices. Precise control over size, shape, and composition is crucial for tailoring the properties of semiconductor nanostructures for specific applications.

### **How are nanomaterials characterized?**

"Seeing is believing". However, the human eye can see length scales up to 50 – 80 micrometers, almost 50,000 – 80,000 higher than a nanometer. Even objects in nanoscale dimensions cannot be observed using an optical microscope due to the diffraction limit. Nanomaterials are characterized using a variety of techniques

that enable scientists and engineers to understand their structure, composition, morphology, and properties at the nanoscale. Some standard characterization techniques for nanomaterials include:

1. Transmission Electron Microscopy (TEM): TEM allows for the imaging of nanomaterials at extremely high magnification. It involves transmitting an electron beam through a thin sample, providing information about its internal structure, crystal lattice, and atomic arrangement. TEM is useful for studying the morphology, size, defects, and composition of nanomaterials.
2. Scanning Electron Microscopy (SEM): SEM is a widely used technique that provides high-resolution imaging of nanomaterials. It uses a focused electron beam to scan the sample's surface, generating detailed images that reveal the sample's morphology, size, and shape.
3. Atomic Force Microscopy (AFM): AFM is a powerful technique for characterizing nano materials at the atomic and molecular level. It uses a sharp probe to scan the sample surface, measuring the forces between the probe and the material. AFM provides information on topography, roughness, and surface properties with high resolution.
4. Dynamic Light Scattering (DLS): DLS is employed to measure the size distribution and aggregation state of nano materials in a liquid suspension. By analyzing the fluctuations in scattered light intensity caused by Brownian motion, DLS provides information on particle size, size distribution, and stability.
5. X-ray Diffraction (XRD): XRD is employed to determine the crystal structure and phase composition of nanomaterials. By directing X-rays at a sample, XRD measures the angles and intensities of the X-ray diffraction patterns, enabling the identification of crystal structures and lattice parameters. By looking into the width of the diffraction patterns, it is possible to determine the nanocrystallites sizes using Debye Scherer equation.
6. Spectroscopic Techniques: Various spectroscopic methods, such as UV-Vis spectroscopy, fluorescence spectroscopy, and Raman spectroscopy, are utilized to study the optical properties, electronic transitions, and vibrational modes of nanomaterials.
7. Thermogravimetric Analysis (TGA): TGA measures the change in weight of a nanomaterial as a function of temperature. It provides information about its thermal stability, decomposition behavior, and presence of volatile components.
8. Surface Area and Porosity Analysis: Techniques such as Brunauer-Emmett-Teller (BET) analysis and pore size distribution measurements help determine the surface area and porosity of nanomaterials. These parameters are crucial for understanding adsorption/desorption properties and catalytic activity.

These are just a few examples of the many characterization techniques available for nanomaterials. The selection of specific methods depends on the properties and nature of the materials being studied, as well as the desired information to be obtained. Often, a combination of different techniques is employed to gain a comprehensive understanding of nanomaterials.

In the following section, we will discuss a bit more details about quantum dots, which exhibit quantum confinement effects at nanoscale dimensions.

### **What are quantum dots and their size-dependent optoelectronic properties?**

Quantum dots are semiconducting nanoparticles that exhibit quantum confinement effects, which give rise to unique optical and electronic properties due to their nanoscale size. They are typically made of semiconductor materials such as cadmium selenide (CdSe), lead sulfide (PbS), or indium phosphide (InP). The size of quantum dots can range from a few nanometers to several tens of nanometers in diameter.

The properties of quantum dots are governed by quantum mechanics, which leads to discrete energy levels and size-dependent electronic transitions. Due to their small size, quantum dots exhibit a phenomenon called quantum confinement. This means that the motion of electrons and holes within the quantum dot becomes confined, resulting in quantized energy levels. The energy gap between these levels can be precisely controlled by varying the size of the quantum dot, allowing for tunability of their optical and electronic properties.

The bandgap of a material refers to the energy difference between its valence band (the highest energy level occupied by electrons) and its conduction band (the lowest energy level available for electrons to move freely). It determines the energy required for electrons to transition from the valence band to the conduction band, thereby influencing the optical and electronic properties of the material.

In bulk semiconductors, the bandgap is a material-specific property that remains relatively constant. However, in quantum dots, the size of the particle becomes comparable to or smaller than the exciton Bohr radius (the characteristic length scale for electron-hole interactions), resulting in quantum confinement.

As the size of a quantum dot decreases, the confinement of charge carriers within a small volume causes their energy levels to become quantized. This quantization leads to a discrete set of energy levels, often referred to as energy states or electronic shells. The energy spacing between these levels increases as the size of the quantum dot decreases.

The quantized energy levels in quantum dots result in a size-dependent bandgap. Smaller quantum dots exhibit larger bandgaps compared to their bulk counterparts. This phenomenon can be understood as follows: In larger quantum dots, where the dimensions are comparable to the exciton Bohr radius, the energy levels are more closely spaced. As a result, the energy difference between the highest occupied energy level (valence band) and the lowest unoccupied energy level (conduction band) is smaller, corresponding to a smaller bandgap. This is because the confinement of electrons and holes is relatively weak, allowing them to interact more effectively.

Conversely, in smaller quantum dots, the energy levels become more widely separated due to stronger confinement. Consequently, the energy required for electron transitions from the valence band to the conduction band increases, leading to a larger bandgap. The increase in bandgap energy corresponds to a shift towards shorter wavelengths in the absorption and emission spectra of the quantum dots.



By precisely controlling the size and composition of quantum dots, their bandgap energy can be tuned across a wide range of values. This tunability is a highly desirable property, as it allows researchers to engineer quantum dots with specific optical properties and emission colors. It enables the production of quantum dots that emit light across the visible spectrum, from ultraviolet to near-infrared, making them versatile for various applications in optoelectronics, displays, and biomedical imaging.

Additionally, quantum dots have high photoluminescence efficiency, meaning they efficiently convert absorbed light into emitted light, making them attractive for applications requiring bright and vibrant colors. They also exhibit excellent photochemical stability, resistance to photobleaching, and long fluorescence lifetimes.

It is important to note that some quantum dots contain heavy metals, such as cadmium, which raises environmental and health concerns. However, efforts are being made to develop environmentally friendly quantum dots, such as those based on non-toxic materials like indium phosphide and zinc sulfide, to mitigate these concerns and expand their potential applications.

# Nuclear magnetic resonance spectroscopy in materials research

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## I. INTRODUCTION

Many atomic nuclei possess an intrinsic spin ( $I = 1/2, 1, 3/2, 2$  etc.) and hence a magnetic moment  $\mu = \gamma\hbar I$  where  $\gamma$ , the nuclear magnetogyric ratio, is determined by the mass and the charge of the atomic nucleus. In presence of a magnetic field ( $H$ ), the energy  $E = \gamma\hbar I \cdot H$  corresponding to this magnetic moment is split into  $2I + 1$  levels, which is called nuclear Zeeman splitting. For a typical laboratory magnetic field, the separation between the energy levels corresponds to radiofrequency (*rf*) energy lying in the range of 5-1000 MHz. A typical nuclear magnetic resonance (NMR) spectroscopy facility is set up with a magnet that may be an electromagnet for low magnetic fields or a superconducting current magnet for high magnetic fields. The magnet produces a homogeneous magnetic field on a small volume of sample. Simultaneously, the sample is irradiated with a *rf* field that is swept over a suitable range of frequencies ( $\nu$ ). When the *rf* energy ( $= h\nu$ ) is matching with energy of separation between the levels, the nuclei are excited from the lower to the higher energy level, *i.e.*, resonance takes place accompanied by absorption of energy from the *rf* source, which is then detected experimentally.

In a modern day pulsed NMR experiment, a NMR spectrometer produces a *rf* pulse in resonance condition to excite the spin system, *i.e.*, causing a transition of the spin system to an overall higher energy state. The system is then allowed to return to its original thermal equilibrium state through the release of energy which is also monitored in the NMR spectrometer in the form of a signal decaying with time, called the free-induction-decay (FID) signal. The signal is analyzed to obtain, (a) time averaged NMR parameters, such as, shape and position of NMR line or spectrum, and (b) time dependent or dynamic parameters such as NMR spin-spin and spin-lattice relaxation rates. These NMR parameters are determined by the different interactions of the nuclei with their environment or surroundings. The interactions and their experimental manifestations are outlined below.

(i) Solids consist of a large number of nuclei of the order of Avogadro's number. The nuclear magnetic moments interact with each other which is nuclear-nuclear dipolar interaction. It results in the broadening of

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energy levels and so also of the resonance spectrum. Analysis of the spectrum may yield the distribution of the nuclei, and hence the atomic structure of the solid. Moreover, when the nuclei are in a state of some motion often induced by temperature, the nuclear dipolar interaction is averaged out and a narrowing of resonance spectrum should be observed.

(ii) Electron spin and/or orbital magnetic moments that are present in magnetic systems interact with nuclear magnetic moments. Electron-nuclear dipolar interaction causes large broadening of the NMR spectrum. The temperature dependence of spectrum broadening follows that of the magnetization of the sample.

(iii) *s*-electrons in the electron shell of an atom or in the conduction band of a metal have a finite overlap at the nucleus and it produces a local magnetic field over and above the external magnetic field through the *s*-contact hyperfine interaction. This local field is again modified by the spin and orbital magnetic moment of unpaired electrons in paramagnetic materials, and more strongly in ferromagnetic materials. Depending on the magnetization of the sample, the local magnetic field produces a shift in the position of resonance from that of a reference material in which nuclei experience negligible or no local field. In ferromagnetic materials, the local field can be large enough to produce Zeeman splitting such that resonance is obtained even in absence of an external magnetic field.

(iv) Nuclei having spin  $I > 1/2$  possess nuclear electric quadrupole moment which interacts with the electric field gradient in the surroundings produced by the electron charge distribution of neighboring atoms. This interaction acts as a second order perturbation on the Zeeman interaction and causes splitting of resonance spectrum. Analysis of such spectra yields structural information of the system under study.

(v) At resonance, the spin system undergoes excitation from a lower energy state to a higher energy state. It then returns to the original lower state through processes called spin-spin relaxation, *i.e.*, through interaction among the nuclear spins themselves, and also spin-lattice relaxation, *i.e.*, through the interaction of nuclear spins with their environment, namely, the local magnetic field, electric charge distribution, *etc.* Study of the dynamics of the nuclear spin excitation, through the measurements of spin-spin and spin-lattice relaxation rates gives valuable information about the physical properties of the system.

The analysis of NMR data is often aided by the knowledge of atomic structure, *e.g.*, X-ray diffraction (XRD) results and of the magnetic properties of the sample. Some results obtained from NMR experiments involving only the shape and position of resonance spectra are described below.

## II. DISORDER IN CORE-SHELL STRUCTURE OF COBALT-COPPER (CO-CU) NANOPARTICLE SYSTEM

Chemically prepared granular binary alloys  $\text{Co}_x\text{Cu}_{1-x}$  ( $x = 0.10, 0.32$  and  $0.76$ ) were earlier studied [1] by XRD and electron microscopy and characterized as assemblies of nearly spherical particles of average size 15 nm formed in *fcc* structure. Henceforth these samples will be designated as Co- $x$ , *i.e.*, by their Co content, *viz.*,

Co-0.10, Co-0.32 and Co-0.76. From magnetization measurements, the particles were modeled as having a Co rich ferromagnetic core surrounded by uncompensated dilute Co moments in a Cu rich shell. The electrical resistivity were characteristic of elastic scattering of electrons in a strongly disordered material. Since these samples possessed a large ferromagnetic content, it was possible to observe and analyze  $^{59}\text{Co}$  NMR signal at the liquid helium temperature of 4.2 K, elucidating ferromagnetic Co atoms distribution in this disordered system[2].

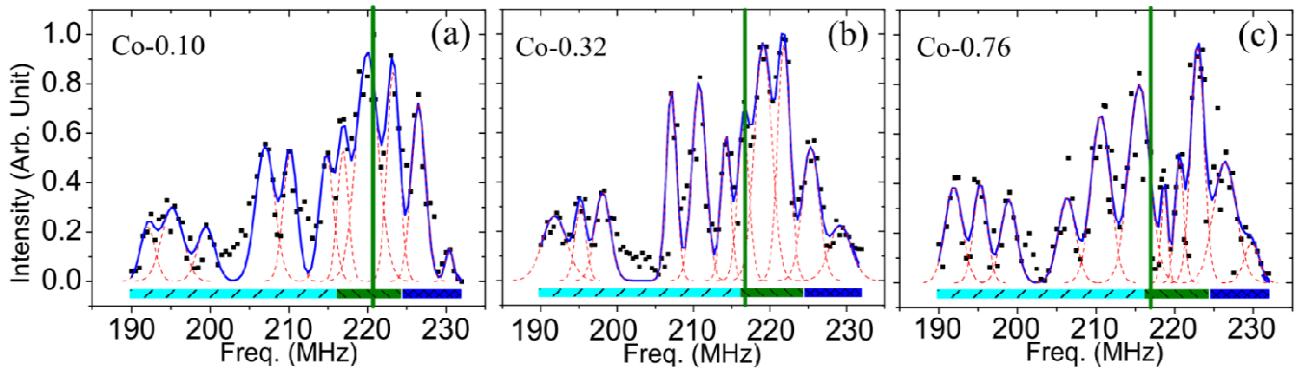


FIG. 1.  $^{59}\text{Co}$  zero field NMR spectra at 4 K of (a) Co-0.10, (b) Co-0.32 and (c) Co-0.76. The experimental data are denoted by (■). The spectra are analyzed by a process known as 'deconvolution' which yields different components (broken lines) and the sum of the components (solid line). The horizontal bars denote the range of  $^{59}\text{Co}$  resonance frequencies corresponding to, from right to left, *hcp* Co, *fcc* Co, and Co-Cu environments. In each panel, the vertical solid line divides the area under the spectrum in two equal parts.

In the spectrum of Co-0.1 (Fig. 1 (a)), the resonance is strongest around 220 MHz. Analysis shows that this signal is from Co atoms in the periphery of a *fcc* Co cluster experiencing lattice mismatch with the surrounding Cu environment, while the main *fcc* Co peak is at 223.3 MHz. In Co-0.1 and Co-0.32, both the main and the strained *fcc* Co peaks show similar intensities indicating that a large fraction of Co atoms are at the periphery of clusters. The part of signal at 225 MHz and beyond confirms the presence of *hcp* Co phase that may also evolve as a stacking fault over *fcc* phase. The *hcp* phase could not be identified by earlier XRD studies. The peak at 226.5 MHz is attributed to Co atoms along the c-axis of *hcp* Co, and the 230.4 MHz peak arises from Co in *c*-plane.

In Co-0.1, the deconvolution yields peaks also at 192.1, 195.2, 199.5, 207, 210.2, 214.8 and 216.9 MHz. It was found in Co-Cu alloys that for every substitution in the nearest-neighbor (*NN*) shell of a cobalt atom by a copper atom, the resonance frequency of that particular cobalt is reduced by 16-18 MHz. In a system of cobalt atoms having a varying number of Cu atoms substitutions in their *NN* shells, the resonance spectrum yields satellite peaks along with the main *fcc* peak. Thus, in the spectrum of Fig. 1(a), 207 and 192.1 MHz peaks are assigned as satellites of 223.3 MHz peak, *i.e.*, they are from *fcc* phase Co atoms, but in their *NN* shell, 1 Co atom and 2 Co atoms, respectively, are replaced by Cu. Similarly, 210.2 and 195.2 MHz signals are related to

226.5 MHz signals, *i.e.*, they originate from substitution of 1- and 2 Co atoms by Cu in the NN shell of Co along the c-axis in *hcp* phase. The 214.8 and 199.5 MHz peaks are related to the peak at 230.4 MHz, *i.e.*, arising from Co atoms in *c*-plane of *hcp* Co but with 1- and 2 atoms among the *NN* atoms replaced by Cu. The remaining small peak centered at  $\square$  216.9 MHz almost coincides with the position of the magnetic domain wall signal of *fcc* Co. Fig. 1(b) and (c) can also be described in a similar manner. A modelling based on this NMR experiment shows that the core comprising about 20 % of the volume of the clusters dominates in the ferromagnetism of the particles.

### III. DEFECT INDUCED ROOM TEMPERATURE FERROMAGNETISM IN ORGANIC PEROVSKITE $\text{CH}_3\text{NH}_3\text{PbI}_3$

Methylammonium lead iodide is well known in the field of optoelectronics for its excellent photovoltaic properties and extraordinary optical and electronic properties. It has been established that ionic conductivity arises from defects in the form of intrinsic cationic ( $\text{CH}_3\text{NH}_3^+$ ; henceforth labelled as  $MA^+$ ) and anionic ( $\text{I}^-$ ) vacancies. Magnetization and  $^1\text{H}$  NMR measurements in polycrystalline  $\text{MAPbI}_3$  have shown [3] room temperature ferromagnetism providing a real boost for its potential in the field of multiferroics for spintronic application.

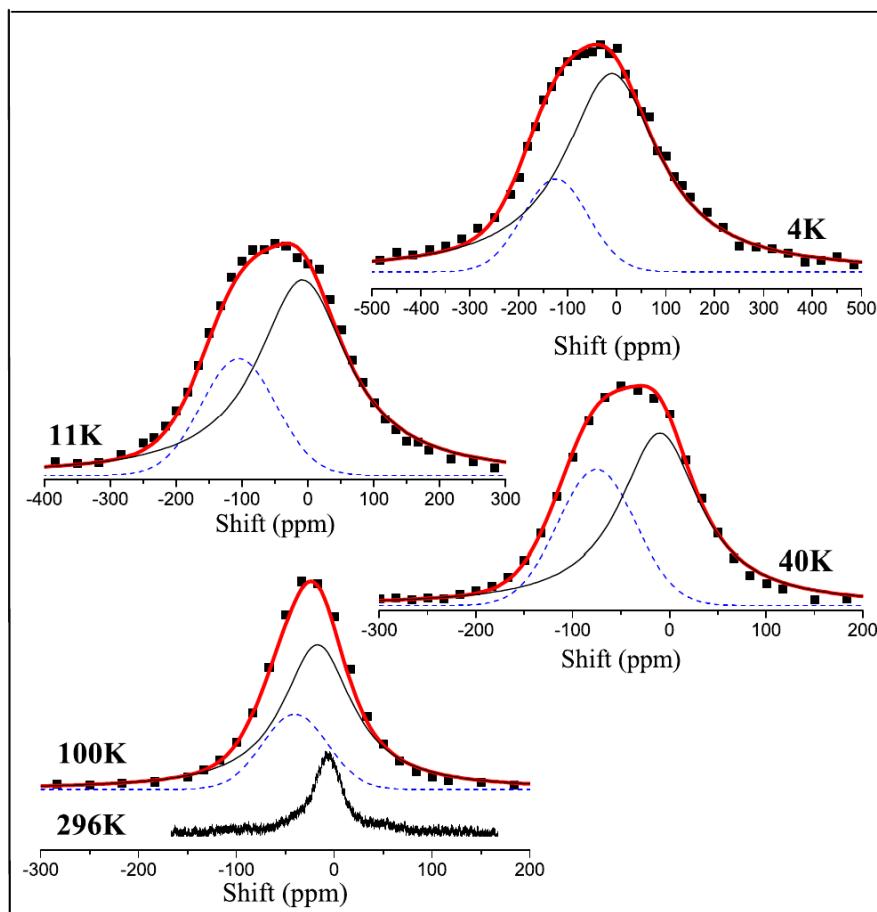


FIG. 2.  $^1\text{H}$  NMR spectra of  $\text{MAPbI}_3$  at different temperatures and their simulation as described in the text. The thin solid and broken lines indicate the resonance components, 'A' and 'B', respectively, and the thick

line denotes their sum.

Fig. 2 shows the  $^1\text{H}$  spectra of  $\text{MAPbI}_3$  at different temperatures 4–296 K. With the lowering of temperature, the spectra showed an apparent shift towards lower frequency and clearly revealed an asymmetric broadening. Below  $\square 150$  K, the spectra could be satisfactorily simulated as a sum of two components; one with a small low frequency shift which is designated as component ‘A’, and another Gaussian resonance component with a larger low frequency shift, denoted as component ‘B’. The simulations are also shown in Fig. 2. Both the components exhibit a pronounced broadening only at low temperatures below  $\square 40$  K. The component A appears to be in the same position irrespective of temperature. The low frequency shift of component B shows a pronounced temperature dependence. By comparing the analyses of magnetization data and NMR spectra, it is reasonably argued that the NMR spectrum component having the larger shift, *i.e.*, component A results from ferromagnetism of  $\text{MAPbI}_3$  while component B corresponds to  $^1\text{H}$  in paramagnetic-like  $\text{MAPbI}_3$ .

$^1\text{H}$  spin-lattice relaxation rate measurements (not described here) have also shown simultaneous existence of two magnetic components with different relaxation rates; the faster one corresponds to the ferromagnetic component, and the other one which is slower by an order of magnitude corresponds to the paramagnetic component.

#### IV CONCLUSION

In condensed matter physics experiments, NMR spectroscopy is a well-known hazards-free technique in which a nuclear property, namely, its spin magnetic moment, is utilized to study various interesting physico-chemical phenomena that are entirely determined by the electron behavior in solid state materials.

#### ACKNOWLEDGMENTS

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## Applications of Computational Methods to Physics and Chemistry

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Now-a-days scientific research is divided into two important fields - one is academic and the other is application. Application field is growing very fast as it has vast applications starting from industry to environment and then to astrophysics. In this regard, research in application field plays a vital role in society. In recent years, computational methods are being applied energetically to different branches of science. We have applied Density Functional Theory (DFT) as well as highly correlated Coupled Cluster (CC) methods to solve research problems in the fields of physics and chemistry. Some of the research areas are discussed here.

Hydrogen ( $H_2$ ) is considered to be an alternative energy carrier as the non-renewable energy resources deplete rapidly due to the sky-rocketing growth of world's population. Besides, burning of fossil fuel leads to harmful emissions which are also responsible for global warming. So,  $H_2$  has drawn significant attention as a next-generation clean energy fuel for mobile and stationary power sources due to its several advantages over other chemical energy carriers. It is one of the most abundant resources found on our planet and devoid of any harmful emission on burning. However, due to its diffusive and buoyant nature, the true challenge lies in either designing efficient hydrogen storage systems with high gravimetric and volumetric hydrogen contents or looking into appropriate chemical reactions which release  $H_2$  on demand at moderate temperatures. Theoretical modelling of the suitable adsorbent systems as well as deeper understanding of the dehydrogenation mechanism of small molecules having E-H (E: N, B) sigma bonds or Ammonia-Borane ( $NH_3BH_3$ ) systems are on the cards in this regard.

Preparation of ester is one of the most important reactions in organic chemistry. The most traditional method of synthesis of ester involves the reaction of a carboxylic acid or its derivatives of acid chloride or acid anhydride with an alcohol in presence of Bronsted acids like HCl, NaHSO<sub>4</sub>, HBF<sub>4</sub>, H<sub>2</sub>SO<sub>4</sub>, H<sub>3</sub>PO<sub>4</sub>, AcOH etc. In recent years, dehydrogenative coupling of two alcohols to make ester in presence of different transition metal catalysts is becoming popular, as this process is quite simple and environment friendly than the conventional methods. In this regard, transition metal-pincer catalysts have been found to be highly effective in lowering the activation barriers of such high-energy demanding reactions. PNP-pincer complexes like

Ru(PNP), Rh(PNP<sup>+</sup>) and Os(PNP) have been employed as catalysts to carryout the formation of esters from primary alcohols.

Within the last two decades, fullerene cages have emerged to be one of the fascinating carbon nanostructures of low dimensions, having captivating physical and chemical properties. These materials display novel properties and are believed to have potential use in many different fields covering from material science to biological science. Fullerenes are carbon clusters in the form of a hollow sphere represented as C<sub>n</sub>, where n is the total number of carbon atoms present in the structure. Topologically the number of isomers of a particular fullerene cage rises with increasing number of carbon atoms (Euler's Theorem). According to Kroto, all the stable fullerenes are those in which no two pentagons share an edge as the pentagon-fusions enhance local strain to destabilize the fullerene cages. This idea has now been widely accepted as the Isolated Pentagon Rule (IPR). For IPR cages, two types of C-C connectivities appear, i.e., [6, 6] (situated between two hexagonal rings) and [6, 5] (between a hexagonal and a pentagonal ring). For Non-IPR cages, extra [5, 5] bonding is observed at the junction of two five-membered rings, which is chemically reactive with larger negative bond resonance energy. In recent years, fullerene functionalization, i.e., endohedral as well as exohedral functionalizations have gained momentum due to potential applications in different scientific areas. Here, metallofullerenes need a special introduction which contains atom/metal-cluster/small molecules in the interior cavity of fullerenes cages. Exohedral functionalization of endohedral metallofullerenes largely depends on the interplay between inside and outside moieties.

Since 1980s, the journey of the term “Agostic” continues even today with enduring interest regarding its nature and conventional symptoms. An agostic bond is a kind of 3c–2e bonding interaction that differs from conventional 3c–4e hydrogen bond. Generally, an intra-molecular interaction between C–H sigma bond (donor orbital) and any closely lying empty metal MOs (acceptor orbital) of same symmetry as well as comparable energy is defined as the agostic interaction. Not only the transition metals (especially d<sup>0</sup> and d<sup>8</sup> systems) but also alkali metals (particularly Li) as well as the lanthanides (especially La, Y) exhibit this kind of interaction. Recently, different types of agostic interactions are coined, i.e., α-agostic, β-agostic, γ-agostic, and ε-agostic which influences different types of elimination, polymerization, insertion and related reactions.

Since the invention of the laser, nonlinear optics (NLO) has emerged as an interesting field of research owing to its potential application in the field of optical communications, data storage, data processing, bio-imaging, optical switch and so on. With the massive progress in optical research, designing optoelectronic devices based on nonlinear optical (NLO) materials has witnessed outstanding development. Molecular systems having large non-linear responses are of great importance as they can be used as high-performance photonic devices. Organic moieties having extensive π conjugation exhibit large NLO responses. Optical responses of these molecules can be tuned as their structure can be chemically modified easily and this is quite helpful for industrial purposes as these molecules can meet the desired design requirement; additionally, these materials have fast switching times. Other than the organic materials, several other materials such as inorganic

materials, different kinds of nanomaterials including organic and inorganic nanocages, electride materials, and so on are also reported to exhibit NLO responses. Due to the versatile potential of NLO molecules, various molecular tailoring techniques have been carried out both theoretically and experimentally to design highly responsive NLO materials and the search for novel NLO materials is still going on.

Superhalogens are unique class of compounds whose electron affinities (EAs) are higher than that of the halogen atoms whereas superalkalis are special type of molecules having ionization energies (IEs) lower than that of the alkali metals. Due to their high electron affinities and excellent oxidizing ability superhalogens have widespread applications. These species have been employed for the oxidation of compounds having very high IEs. Superhalogens have been used as a building block of superacids, electrolytes in Li-ion batteries, ionic liquids, etc. Superalkalis also play a very important role in chemistry owing to their exceptional reducing capability and very low ionization energies. Superalkalis have been used in reducing compounds possessing very low EAs. These species have been employed in the designing of novel alkalides, superbases, hydrogen storage materials, etc. Using superhalogens and superalkalis a new class of salt namely supersalts have been designed with unusual properties such as very high non-linear optical responses. Because of their enormous applications superhalogens and superalkalis have emerged as important research field. We have explored the possibility of formation of stable ionized complexes between coinage metal containing superhalogens ( $\text{AuF}_4$  and  $\text{AuF}_6$ ) and some moderately reactive molecules ( $\text{SiO}_2$ ,  $\text{NH}_3$ ,  $\text{H}_2\text{O}$ ,  $\text{CO}_2$ ,  $\text{CHCl}_3$  and  $\text{CCl}_2\text{F}_2$ ) at density functional theory (DFT) level. Employing DFT, the interaction of four moderately reactive molecules such as benzene, water, ammonia and silicon dioxide with three organic superhalogens has also been investigated. We have studied the reduction of  $\text{SO}_2$  using the superalkalis,  $\text{FLi}_2$ ,  $\text{OLi}_3$  and  $\text{NLi}_4$  at DFT level. We have designed metal-free organic superalkalis by rational modification of benzene using the aforesaid method. Currently, we are trying to design new superhalogens, superalkalis and supersalts for potential applications as mentioned earlier.

Metal-bearing molecules are predicted to be produced under thermodynamic chemical equilibrium near the photosphere of carbon-rich evolved stars. Some of the metal halides were detected more than three decades ago in the circumstellar envelope (CSE) of the carbon-rich star envelope IRC+10216. Metal halide species are generally found near the stellar photosphere. However, metal-cyanides and isocyanides are found to arise from a thin radius where many reactive species such as the carbon chain radicals  $\text{C}_5\text{H}$ ,  $\text{C}_6\text{H}$ ,  $\text{C}_7\text{H}$ , and  $\text{C}_8\text{H}$  are also detected. Mass spectra and experimental findings of important metal clusters found in space, like  $\text{Mg}_m\text{C}_n\text{H}_x$  and  $\text{Be}_m\text{C}_n\text{H}_x$  clusters are in good agreement with the theoretical calculations. On that perspective, calculations of relative energy of different isomers of  $\text{CaC}_6\text{H}_2$  molecule using Density Functional Theory (DFT), MP2 and Coupled Cluster (CC) methods have been performed along with prediction of different important spectroscopic and molecular properties. The study of energetics and spectroscopic properties of the isomers is interesting because a comparative analysis provides an opportunity to understand the chemical processes that lead to their formation in star.

# Macromolecular X-ray Crystallography and Use of Synchrotron Radiation

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## Introduction to macromolecular crystallography

The Discovery in X-ray Crystallography and its application for solving structures of molecules was made by Sir William Bragg and his son, Sir Lawrence Bragg. Their achievements in X-ray Crystallography were recognized and awarded the Noble Prize in 1915.

Protein Crystallography can trace its origin back in 1934 when J.D. Bernal and Dorothy Crowfoot Hodking at the Cavendish Laboratory in Cambridge (U.K) discovered that crystals of the stomach protease pepsin yielded an X-ray diffraction pattern. The first protein structure of Myoglobin was published by Kendrew, Dickerson and Strandberg in Nature in 1960.

To get atomic structure from diffraction pattern in the early days was a very slow and painstaking process upto 1970. Advancement in computing power for fast calculation and graphics and molecular biology have dramatically speeded up the process with new protein structures and deposited in *Protein DataBank*. From its slow birth in the sixties, protein Crystallography has now matured into an exciting and powerful technology. It is still moving at an accelerating pace as evidence from the development of new methodologies in molecular biology and biochemistry. The widespread availability of computer power for fast calculation in structure determination with graphics, have supported the striking growth in crystallography and in crystallographic studies of biological relevance, structural genomics and fulfilled the needs of the pharmaceutical industry.

A rapid growth came from the increased access to synchrotron sources, which resulted in new ways of collecting X-ray diffraction data and allowed novel structure determination techniques.

This open access data collection from Synchrotron radiation/sources, together with the use of efficient X-ray detectors, is probably the reason of exponential growth of this field in the studies of structural biology during last few years. From the use of third generation synchrotron X-ray sources, more than 100000 protein structures were determined at about 2Å resolution. And such type of protein data bank is available today.

With this achievement, the structural biologists are shifting their field of interest from determination of static structures to elucidating dynamic aspects of protein function. These aspects are time resolved crystallography

where a biological function is triggered in the crystal with an object to capture molecules in action and determining protein kinetics and structures of intermediate states.

In the study of reversible, light initiated reactions, 100ps time resolution at synchrotron X-Ray source is used now. The advent of the new free electron lasers for hard x-rays (XFELS: 5-20 Kev) provide high intense, femtosecond x-ray pulses. So, exploration of ultra-fast event, in structural biology/protein enzymes field becomes possible in high resolution synchrotron radiation and XFELS at present days.

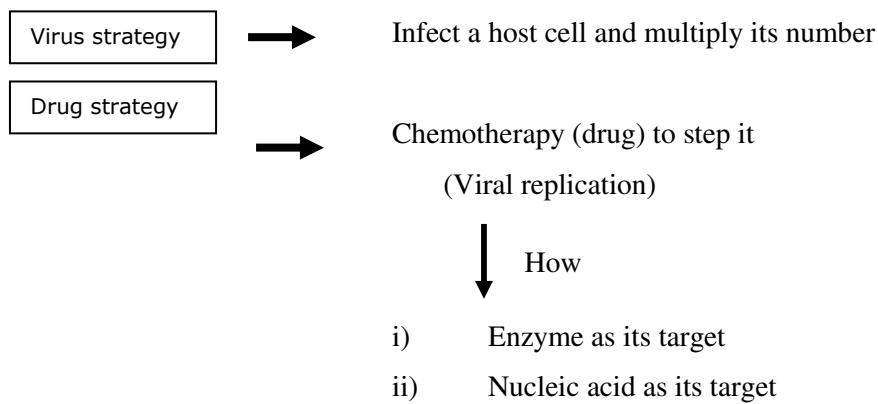
Macromolecular Crystallography, in fact the only, established method for determining the 3D structure of globular proteins, tRNA- and even larger molecular aggregates like viruses. At present, it has now developed into a vast and well-organized subject.

Advances in molecular biology and protein crystallography have yielded a much more promising method which is termed Rational or structure Based Drug Design (SBDD). Decades of research have demonstrated that the proteins are the site of action (target) (Flow chart 1) for most of the drugs. In this method, key proteins are identified, crystallized and then their crystal structures determined. Through the use of interactive computer graphics and molecular modeling software it is possible to design potential drugs. This highly interesting field is expanded over several years not only in academic laboratories but also in the pharmaceutical industry.

Now-a-days, many information of living cell has come out from the X-ray Crystallographic studies of protein-inhibitor complex at molecular level. So, as I stated (above), with this available knowledge and information (protein data bank) many pharmaceutical companies are developing drugs of cancer, AIDS etc. As for example, modified nucleosides are potent inhibitors of replication of the retro-viruses via interference with the reverse transcriptase (RT). The viral DNA synthesis (flow chart -1) is stopped and then viral diseases are controlled. Another recent application of protein crystallography is in the field of structural genomics. Biologists are engaged to decipher the function of all the proteins in human body by utilizing variety of highly powerful tools including x-ray protein crystallography.

### **PRINCIPLE OF CHEMOTHERAPY IN VIRAL INFECTION**

Virus genes need regulatory proteins for replication. Nucleoside analogs are potent inhibitors of replication of virus via interference with the enzyme.



Or we can say :-

- i) Drug (Nucleic acid analogs) may attack enzyme and block specific sites of enzyme and make it functionless. Thus, no virus multiplication is possible.
- ii) Drugs (Nucleic acid analogs) may incorporate into viral DNA via nucleoside triphosphate and befools the system, DNA takes it as regular member but being a nonsense coder, the viral DNA synthesis is stopped.

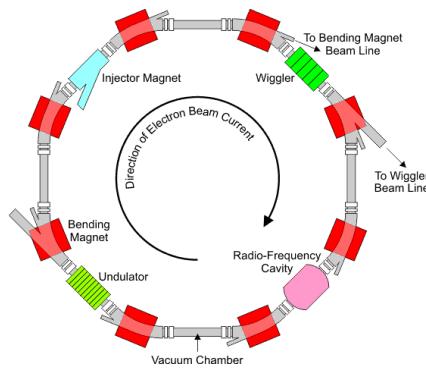
### (Flow Chart – 1)

#### Use of synchrotron radiation

During X-ray diffraction, we Know only a fraction of the energy of the electron is converted to X-rays and the remainder being dissipated as heat. For more intense X-rays, the rotating anode can be used for rapid dissipation of heat from anode for protein crystallography. Due to this heating effect protein crystals damage, and / or the formation of free radicals that can transmit their damaging effects through the solvent channels that run through protein crystals. This effect can be minimized by flash-freezing crystals to about 100<sup>0</sup>K using a nitrogen stream – this is known as cryo-crystallography.

At present, in protein Crystallography, more intense source i.e., Synchrotron radiation is widely used for diffraction datacollection from very small crystal. In this process, electrons are accelerated close to speed of light by a linear accelerator before being injected into a synchrotron ring where the electrons are kept in a circular orbit through the use of high energy magnets. As the electron circle around the ring, they emit electromagnetic energy at a tangent to their orbit. This energy is funneled down beam lines. X-Ray produced at synchrotron beam lines have high intensity and increase in resolution over those available with laboratory sources. It allows diffraction data collection from very small crystal (30-40 micrometers or less) and in a small-time scale. And this enhances the feasibilities of getting structures for an unstable crystal.

Currently third-generation synchrotron radiation source (SRS) are typically heavily based upon the ‘insertion devices’, when straight sections in the storage ring are used for inserting periodic magnetic structures (composed of many magnets that have a special repeating row of N and S poles) that force the electrons into sinusoidal path or helical path. Thus, instead of a single bend, many tens or hundreds of “wiggler” at preciously calculated positions add up or multiply the total intensity that is seen at the end of the straight section. These devices are called wigglers.



There are openings in the storage ring to let the radiation exist and follow a beamline into the experimenter's vacuum chamber where samples are placed in the line of the radiation and detectors are positioned to measure resulting diffraction data. The design of the beamline will vary with the application. High intensity of SRS is specially needed in virus crystallography where the unit cells are very large (rhinovirus by Rossman and Erikson, 1983) and also applicable for small unit cell (Eisenberg et al, 1984). There are several synchrotron radiation sources in the world which have beamline dedicated to protein crystallography and small-angle scattering of X-Ray (SAXS). Examples of available source are the EMBL Laboratory at DESY, Hamburg, EMBL at the European Synchrotron Radiation facility (ESRF) in Grenoble, the Photon Factory in Japan, Advanced Photon Source at the Argonne National Laboratory, Chicago, or the Stanford Synchrotron Radiation Light source. In our country, at least twenty research groups exist who are doing structural biology by using crystallography as a tool in their research. Protein crystallographers of our country have an access to use beamline in abroad like BM14 beamline at ESRF, Grenoble, France through the Department of Biotechnology, Government of India.

#### References:

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