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AN INSTITUTION OF NATIONAL IMPORTANCE ESTABLISHED BY AN ACT OF PARLIAMENT

Dr. Manasi Ghosh
Assistant Professor
Department of Physics (MMV Section)

Curriculum Vitae of Dr. Manasi Ghosh

Area of Research

- Probing molecular dynamics of Pharmaceutical cocrystals by solid state NMR measurements.
- Determination of the structure-activity relationship of the drug molecules.
- Study the structure and dynamics of bio-polymer.
- Analyze the polymorphism of Bio-molecules by NMR crystallography.
- Structural characterization of glass compounds by applying sophisticated solid state NMR methodologies.

Current Affiliation

Assistant Professor, Physics Section, MMV,
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Qualification

M.Sc. in Physics from University of Burdwan
PhD in Physics from Saha Institute of Nuclear Physics
Thesis Title: Experimental Study of the Magnetic Properties of the Low-Dimensional Spin-Trimer Compounds by NMR measurements

A short rationale:

- Dr.Manasi Ghosh, in collaboration with her peers, is presently engrossed in investigating the nuclear spin dynamics and the structure-activity correlation of drug molecules through the measurement of the Chemical Shift Anisotropy (CSA) tensor, site-specific relaxation time, and molecular correlation time. These analytical techniques serve as a key illuminator in the path of drug discovery. Additionally, Dr.Ghosh 's research aims to identify and scrutinize the changes that transpire in the structure and dynamics of various polymorphic states of bio-molecules, employing solid-state NMR methodology. Such an approach holds significant potential in the realm of the Pharmaceutical Industry.

- Cocrystals exhibit diverse dielectric responses under an alternating current (ac) and external electric field, which can be elucidated by the strength and nature of charge-transfer interactions within the cocrystal assembly. The rigid supramolecular framework of strong charge-transfer cocrystals contrasts with the relaxed dynamics of weakly bound charge-transfer complexes, resulting in distinctive dielectric properties. Advanced analytical techniques such as Chemical Shift Anisotropy parameters, spin-lattice relaxation, and molecular correlation times obtained from ^{13}C solid-state NMR spectroscopy measurements provide a deeper understanding of the atomic-scale molecular dynamics within the cocrystals.

- The investigation of molecular dynamics in the amorphous and crystalline phases of biopolymers is currently underway, employing measurements of site-specific spin-lattice relaxation time and molecular correlation time. These endeavors, which establish a correlation between the structure and dynamics of biopolymers, promise to pave the way for the development of innovative bio-mimetic materials. Such materials hold immense potential in the fields of Tissue Engineering and Pharmaceutical Industries.

Outcomes of research

- The acquisition of data pertaining to the electronic configuration and spin dynamics at different crystallographic sites of drug molecules will greatly advance the field of "NMR crystallography." Moreover, such information will facilitate the development of effective strategies for antifungal drug administration by furnishing a comprehensive understanding of the structure and dynamics of diverse segments of the drug molecule.
- Detailed examination of the electronic configuration and nuclear spin dynamics at various carbon nuclei sites of biopolymers at the atomic scale is poised to revolutionize the design of biomimetic materials. These materials find broad applications across several industries, including but not limited to, food technology, pharmaceuticals, textile printing, and material science.
- Solid-state NMR spectroscopy measurements have confirmed the existence of molecular dynamics at the atomistic scale of cocrystals. An established theory proposes that the rotation of molecules within a crystal can heighten the dielectric constant of organic materials (orientational polarizibility). Remarkably, the rotational local correlation time has now been measured through 13C solid-state NMR spectroscopy, representing a significant achievement, as Deuterium NMR spectroscopy is typically utilized for this purpose. This measurement confirms the theoretical basis for this phenomenon.

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Impact on Society

Sophisticated NMR methodologies hold the key to unraveling the structure-activity relationship of drug molecules and illuminating the path of drug discovery. Furthermore, these studies are essential for comprehending the electronic distribution around a nucleus and nuclear spin dynamics at various regions of the drug molecule, thereby enabling the development of effective drug administration strategies.

An investigation of the local electronic environment and nuclear spin dynamics at crystallographically distinct carbon nuclei sites of biopolymers through CSA measurements and spin-lattice relaxation time measurements promises to reveal biomimetic materials. Such materials are of immense interest to Tissue Engineering and Pharmaceutical Industries. Additionally, these studies will significantly enhance the field of "NMR-crystallography."

Vision of the Researcher

The development of a comprehensive structure and dynamics database for key drug molecules through the NMR crystallographic approach promises to advance drug discovery and design endeavors. This database would contain detailed information about the electronic configuration and nuclear spin dynamics of the drug molecules, providing a robust understanding of their three-dimensional structures and properties. The potential benefits of this approach extend to the development of novel drug delivery strategies and the enhancement of drug efficacy through targeted delivery. Moreover, the database can be utilized to gain insights into the mechanism of drug action and improve the rational design of drug molecules. Thus, this initiative holds tremendous promise for advancing drug discovery efforts and ultimately contributing to improved public health outcomes.

Funded Projects

SERB-POWER Grant (File No: SPG/2021/000303) (ongoing)
Title: NMR Crystallographic Approach to Analyze the Polymorphism of Bio-molecule.
Fund amount: Rs. 5995264

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IoE-BHU Grant (Dev. Scheme No. 6031) (ongoing)
Title: Determination of the Structure and Dynamics of Drug Molecules
Fund amount: Rs. 1100000

SERB-DST (File No: EMR/2016/000249)(completed)
Title: Study of the magnetic properties and low frequency spin-dynamics of two-dimensional spin-1/2 honeycomb lattice compounds by NMR measurements.
Fund amount: Rs. 4322560

UGC- Start-up Grant(No.F.30-12/2014(BSR)) (completed)
Title: Experimental Investigation of the Spin-dynamics of low-dimensional antiferromagnetic-antiferromagnetic-ferromagnetic (AAF) spin chain Compounds
Fund amount: Rs. 600000

Five Best Publications

1. R. Bhowal, A. Balaraman, **M. Ghosh***, S. Dutta*, K. K. Dey*, D. Chopra*, "Probing Atomistic Behavior to Unravel Dielectric Phenomena in Charge Transfer Cocrystals", *Journal of American Chemical Society*, 2021, **143**, 1024-1037. (Corresponding author) https://dx.doi.org/10.1021/jacs.0c11459
2. Indrajeet Mandal, Shweta R. Keshri, Lekhan Lodhi, Krishna Kishor Dey, Manasi Ghosh, Aswini Ghosh, Amarnath R. Allu, "Correlation of structure and ionic-conductivity in phosphate glass using MAS-NMR and impedance spectroscopy: Influence of sodium salt." *Physical Review Materials*, 2022, **6**, 115403. (Corresponding author) https://doi.org/10.1103/PhysRevMaterials.6.115403
3. K. K. Dey, **M. Ghosh**, Understanding the Effect of an Anionic Side-Chain on the Nuclear Spin Dynamics of a Polysaccharide, *Cellulose*2022, **29**, 1381–1392. (Corresponding author) https://doi.org/10.1007/s10570-021-04394-5
4. LekhanLodhi, Jai PrakashYadav, Toshio Yamazaki, Nghia Tuan Duong, Srinivasa L. Poojary, Krishna KishorDey, Yusuke Nishiyama, **ManasiGhosh**, "NMR Crystallographic Approach to Study the Variation of the Dynamics of Quinine and its Quasienantimer Quinidine," *The Journal of Physical Chemistry* C, 2022, **126**, 17291-17305. (corresponding author) https://doi.org/10.1021/acs.jpcc.2c04470
5. K. K. Dey, **M. Ghosh***, "Determination of Chemical Shift Anisotropy Tensor and Molecular Correlation Time of Proton Pump Inhibitor Omeprazole by Solid State NMR Measurements", *New Journal of Chemistry*, 2020, **44**, 19393. (Corresponding author) DOI: 10.1039/d0nj01827a

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List of Publications

1. Rajat Kumar Mishra, Savita Kumari, Prince Sen, Sarvesh Kumar Avinashi, Harel Thomas, Zaireen Fatima, **Manasi Ghosh**, Krishna Kishor Dey, Chandkiram R Gautam, "Doping Impacts of La2O3 on Physical, Structural, Optical and Radiation Shielding Properties of (30-x) BaCO3-30TiO2-40SiO2-xLa2O3 (0≤ x≤ 6) Glasses for Optoelectronic Applications, "*Physica Scripta*, 2023, 98, 105918 (Co-author) DOI 10.1088/1402-4896/acf539.
2. Prince Sen, Bijay Laxmi Pradhan, Lekhan Lodhi, **Manasi Ghosh**, Krishna Kishor Dey, "Precise Measurement of Qn Species Distributions in Modified Silicate Glass Using Phase-Adjusted Spinning Sideband NMR Experiment," *Silicon*, 2023, 1-7. (Corresponding author) https://doi.org/10.1007/s12633-023-02639-5
3. Bijay Laxmi Pradhan, Jai Prakash Yadav, Lekhan Lodhi, Prince Sen, Krishna Kishor Dey, **Manasi Ghosh,** "Atomic-Scale Resolution Insights into Structural and Dynamic Differences between Ofloxacin and Levofloxacin, "*ACS Omega* 2023, 8, 26, 24093-24105.(Corresponding author) https://doi.org/10.1021/acsomega.3c03406
4. Jagannath Gangareddy, Hamad Syed, Saswata Chakraborty, Prince Sen, **Manasi Ghosh**, Krishna Kishor Dey, K Bhattacharyya, K Annapurna, Venugopal Rao Soma, Amarnath R Allu, "Tunable, Efficient, Ultrafast Broadband Nonlinear Optical Properties of TiO2–Loaded Complex Phosphate Glasses," *Materials Research Bulletin*, 2023, **167**, 112414.(Co-author) https://doi.org/10.1016/j.materresbull.2023.112414
5. Rajat Kumar Mishra, Prince Sen, Krishna KishorDey, **ManasiGhosh**, ChandkiramGautam, "Physical, Structural, and Optical Properties of ZrO2 Reinforced (100-x–y)[SrTiO3]-x [2B2O3. SiO2]-y [ZrO2] Glasses, "*Silicon*, 2023, 1-19. (Co-author) https://doi.org/10.1007/s12633-023-02523-2
6. Lekhan Lodhi, Manasi Ghosh, Krishna Kishor Dey, Janak Dulari Ahi, "Analysis of metabolite profiles of haemolymph in developmental stages of the silkmoth with high-resolution nuclear magnetic resonance," *Biologia*, 2023, 1-13.(Co-author) https://doi.org/10.1007/s11756-023-01388-5
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8. Abhishek Madheshiya, Anod Kumar Singh, Rajat Kumar Mishra, Krishna Kishor Dey, Manasi Ghosh, Kamal Kumar Srivastava, Prerna Garg, Chandkiram Gautam, "Synthesis, physical, optical and structural properties of SrTiO3 borosilicate glasses with addition of CrO3 ", *Bulletin of Materials Science*, 2023, **46**, 34. (Coauthor) https://doi.org/10.1007/s12034-022-02871-6

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9. Lekhan Lodhi, Jai Prakash Yadav, Toshio Yamazaki, Nghia Tuan Duong, Srinivasa L. Poojary, Krishna Kishor Dey, Yusuke Nishiyama, **Manasi Ghosh**, "NMR Crystallographic Approach to Study the Variation of the Dynamics of Quinine and its Quasienantimer Quinidine," *The Journal of Physical Chemistry* C, 2022, **126**, 17291-17305. (corresponding author) https://doi.org/10.1021/acs.jpcc.2c04470
10. Jai PrakashYadav, Lekhan Lodhi, Tamseel Fatma, Krishna Kishor Dey, **Manasi Ghosh**, "Investigation of the Influence of Various Functional Groups on the Dynamics of Glucocorticoids." *ACS Omega*, 2022, **7**, 43190-43209 (Corresponding author) https://doi.org/10.1021/acsomega.2c05892
11. Indrajeet Mandal, Shweta R. Keshri, Lekhan Lodhi, Krishna Kishor Dey, Manasi Ghosh, Aswini Ghosh, Amarnath R. Allu, "Correlation of structure and ionic-conductivity in phosphate glass using MAS-NMR and impedance spectroscopy: Influence of sodium salt." Physical Review Materials, 2022, **6**, 115403.(Corresponding author) https://doi.org/10.1103/PhysRevMaterials.6.115403.
12. G. Jagannath, Anuraag Gaddam, S. Venugopal Rao, D.A. Agarkov, G.M. Korableva, Manasi Ghosh, Krishna Kishor Dey, José M.F. Ferreira , Amarnath R. Allu , "Tunable femtosecond nonlinear absorption and optical limiting thresholds of La_2O_3 – B_2O_3 glasses by controlling the borate structuralunits", *Scripta Materialia* 2022, **211**, 114530.(Co-author) https://doi.org/10.1016/j.scriptamat.2022.114530
13. Bandaru Santhosh kumar, Mahendra Birmaram Choudhary, Anup Kumar Bera, Seikh Mohammad Yusuf, Manasi Ghosh, Bholanath Pahari, "High Na^+ conducting $Na_3Zr_2Si_2PO_{12}/Na_2Si_2O_5$ composites as solid electrolytes for Na^+ batteries", *Journal of the American Ceramic Society*, 2022, **105**(7), 5011-5019. (Co-author) https://doi.org/10.1111/jace.18463
14. K. K. Dey, **M. Ghosh**, Understanding the Effect of an Anionic Side-Chain on the Nuclear Spin Dynamics of a Polysaccharide, *Cellulose* 2022 , **29**, 1381–1392.(Corresponding author) https://doi.org/10.1007/s10570-021-04394-5
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21. Krishna Kishor Dey, Shovanlal Gayen, **Manasi Ghosh***,"Structure and dynamics of sodium alginate as elucidated by chemical shift anisotropy and site-specific spin–lattice relaxation time measurements", *European Biophysics Journal*, 2021, **50**(7), 963-977 (Corresponding author) https://doi.org/10.1007/s00249-021-01559-9
22. Krishna Kishor Dey, **Manasi Ghosh***, "Study of the Structure and Dynamics at Various Parts of the Antibacterial Drug Molecule Cefpodoxime proxetil*", Solid State Nuclear Magnetic Resonance,* 2021,**115**, 101752.*(*Corresponding author*)*
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30. K. K. Dey, **M. Ghosh*, "**Understanding the effect of deacetylation on chitin by measuring chemical shift anisotropy tensor and spin lattice relaxation time", *Chemical Physics Letters***,** 2020,**738**, 136782.(Corresponding author)
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Award and Recognition

- Most Productive Researcher Award 2020 from Banaras Hindu University
- GATI-NASI Award 2022 from DST

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