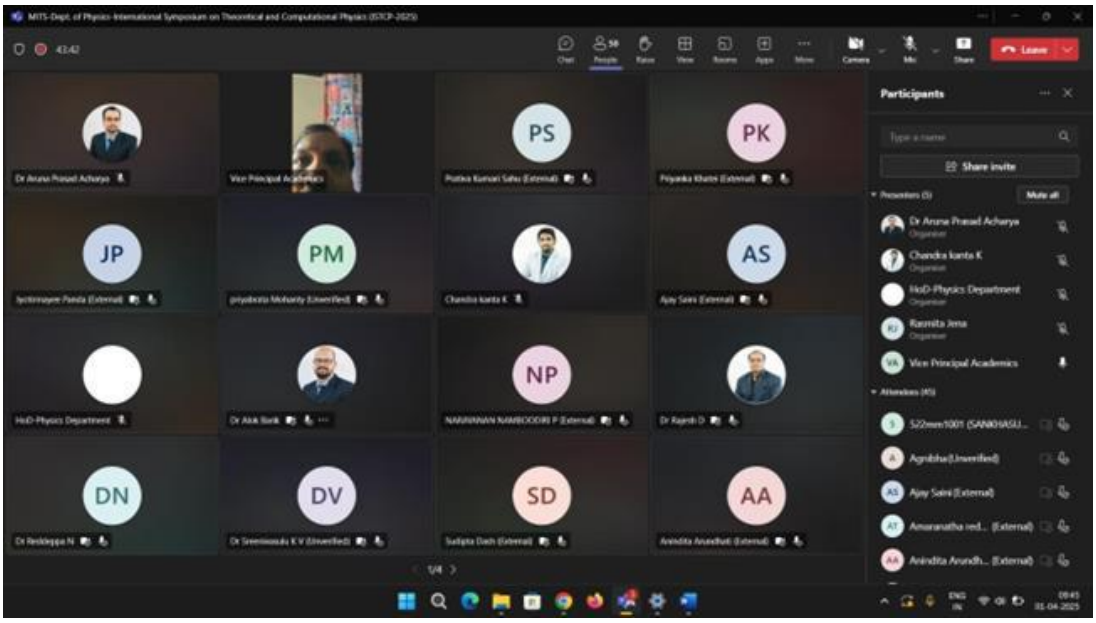
A Report on International Symposium on "Theoretical and Computational Physics (ISTCP-2025)" Organized by Department of Physics from 01.04.2025 to 03.04.2025



Report Submitted by: Dr. Aruna Prasad Acharya, Assistant Professor, Department of Physics.
Mode of Conduct: Online
Report Received on 04.04.2025.

Introduction:

The International Symposium on Theoretical and Computational Physics (ISTCP-2025) was successfully organized by the Department of Physics, MITS, from 1st to 3rd April 2025. The symposium aimed to bring together leading researchers, academicians, and students to discuss cutting-edge advancements in theoretical and computational physics, fostering collaborations and knowledge exchange. The event featured a diverse range of topics, from quantum chromodynamics (QCD) and astrophysics to spintronics and condensed matter physics, with participation from esteemed international and national speakers.

Symposium Overview

- Dates: 1st – 3rd April 2025
- Venue: Online / Virtual Mode
- Organized by: Department of Physics, MITS
- Convener: Dr. Aruna Prasad Acharya
- Session Chairs: Dr. Aruna Prasad Acharya, Dr. K. Chandrakanta, & Dr. Rasmita Jena

Inaugural Session (1st April 2025)

The symposium commenced with a thoughtful inaugural ceremony that set the tone for the academic proceedings to follow. Beginning at G:30 AM, Dr. K. Chandrakanta delivered the opening remarks, establishing the context for the event and inviting participants into a space of collaborative scientific inquiry. At 09:33 AM, Dr. Aruna Prasad Acharya presented the welcome address, underlining the significance of theoretical and computational methods in advancing modern physics. This was followed at 09:38 AM by an inspirational message from Dr. M. Chandra Sekhar, Head of the Department of Physics, who highlighted MITS's unwavering commitment to research excellence. At 09:43 AM, Dr. P. Ramanathan, Vice-Principal of MITS, addressed the audience on the vital role of interdisciplinary research in pushing the frontiers of scientific knowledge. The inaugural session concluded at **09:48 AM** with a vote of thanks by **Dr. K. Chandrakanta**, who expressed sincere appreciation to all dignitaries, speakers, participants, and organizers for their valuable contributions.

Scientific Sessions & Key Discussions

Day 1 (1st April 2025)

Session 1 (Session Chair: Dr. K. Chandrakanta)

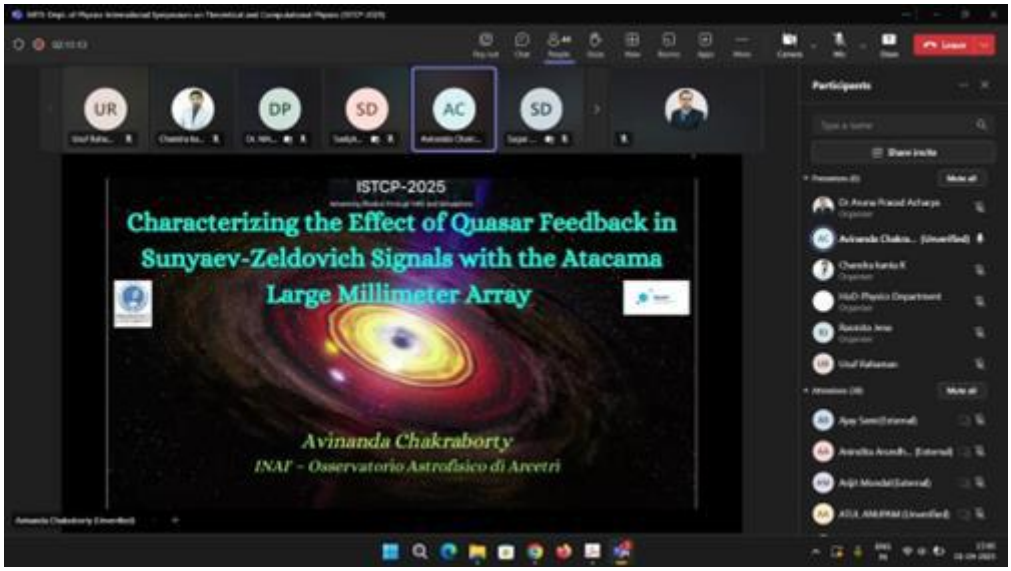
- **10:00 AM – 10:45 AM:** The first talk of the symposium was delivered by Dr. Shreyansh Shankar Dave from Veer Kunwar Singh University, India, on the topic *"Simulating Evolution of Energy Density Fluctuations in QCD Plasma."* In this insightful session, Dr. Dave discussed the thermalization processes of Quantum Chromodynamics (QCD) matter using Fokker-Planck dynamics. His presentation shed light on how energy density fluctuations evolve in the early stages of heavy-ion collisions, offering key implications for understanding experimental results in high-energy nuclear physics.

- **11:00 AM – 11:45 AM**: The second talk was presented by **Dr. Divya Pandey** from the **University of Tartu, Estonia**, on the topic *"Introduction to Observational Astrophysics."* Dr. Pandey offered a comprehensive overview of the key observational techniques used in astrophysics, with a special focus on multi-wavelength approaches. Her talk emphasized how these methods contribute to our understanding of galaxy formation and evolution, providing valuable insights into the large- scale structure of the universe.

- **12:00 PM – 12:45 PM**: The third talk of the day was delivered by **Dr. Md Ramiz Aktar** from **National Tsing Hua University, Taiwan**, on the topic *"Magnetized Accretion Flows Around Black Holes."* Dr. Aktar presented advanced relativistic magnetohydrodynamic (MHD) simulations to explore the complex dynamics of accretion disks surrounding black holes. His talk skillfully bridged theoretical models with recent observational breakthroughs, particularly those from the Event Horizon Telescope, offering deeper insights into the behavior of matter in extreme gravitational environments.

Session 2 (Session Chair: Dr. Aruna Prasad Acharya)

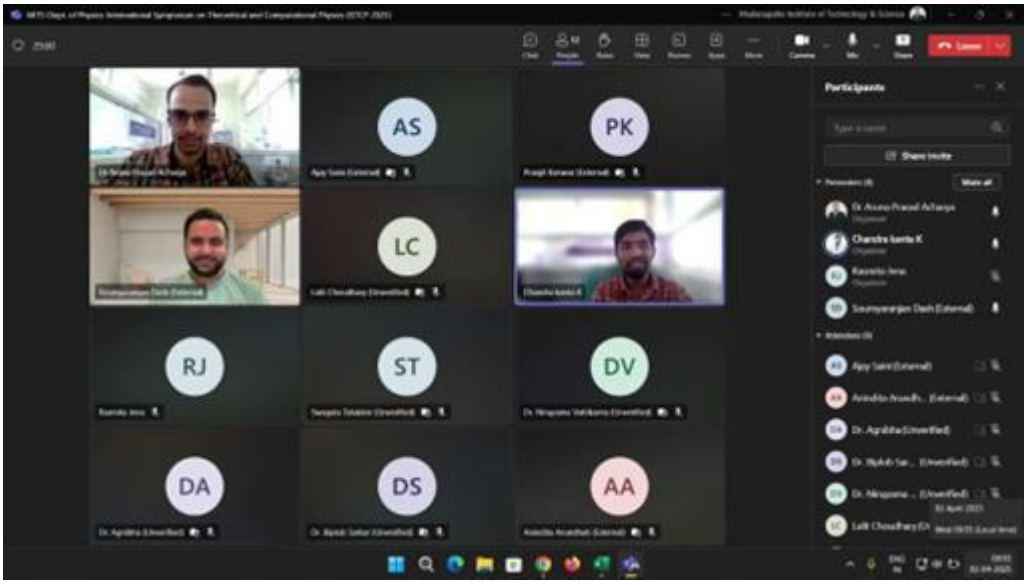
- **2:00 PM – 2:45 PM**: The fourth talk was presented by **Dr. Usuf Rahaman** from **MITS, India**, on the topic *"Relativistic Mean Field (RMF) Theory in Transitional Nuclei (Os & Hg)."* In this engaging session, Dr. Rahaman showcased the effectiveness of RMF theory in exploring nuclear structure, particularly in transitional nuclei. He focused on the phenomenon of shape coexistence inosmium and mercury isotopes, highlighting RMF's strong predictive capabilities and its relevance in understanding complex nuclear configurations.
- **3:00 PM – 3:45 PM**: The fifth talk was delivered by **Dr. Avinanda Chakraborty** from **INAF– Arcetri Observatory, Italy**, on the topic *"Quasar Feedback in Sunyaev-Zeldovich Signals (ALMA Studies)."* Dr. Chakraborty presented results from cosmological simulations investigating how quasar feedback influences the heating of the intergalactic medium. Her talk emphasized the potential of detecting these effects through the Sunyaev-Zeldovich signals using ALMA observations, offering valuable perspectives on the interplay between active galactic nuclei and large-scale cosmic environments.



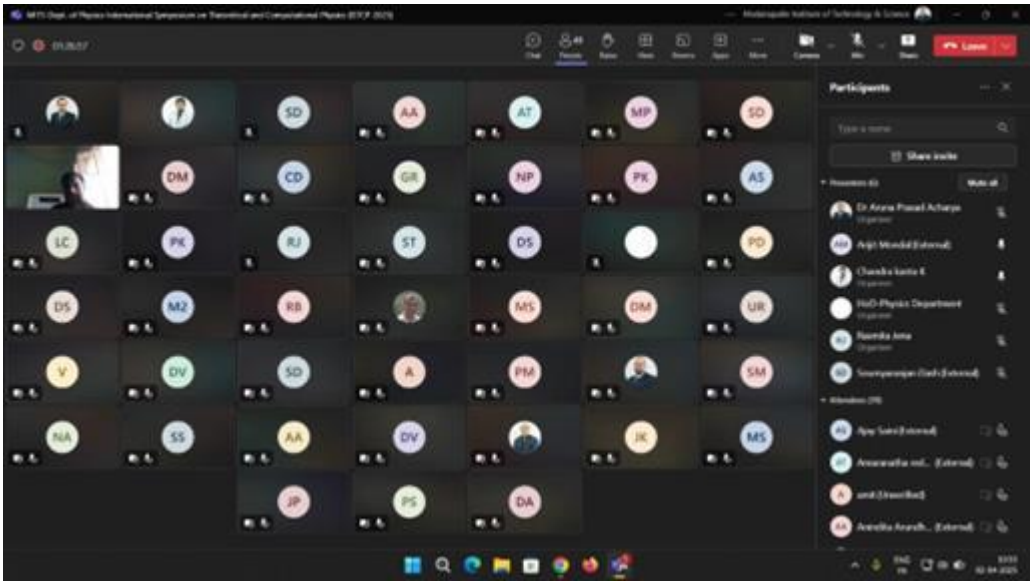
Day 2 (2nd April 2025)

Session 3 (Session Chair: Dr. K. Chandrakanta

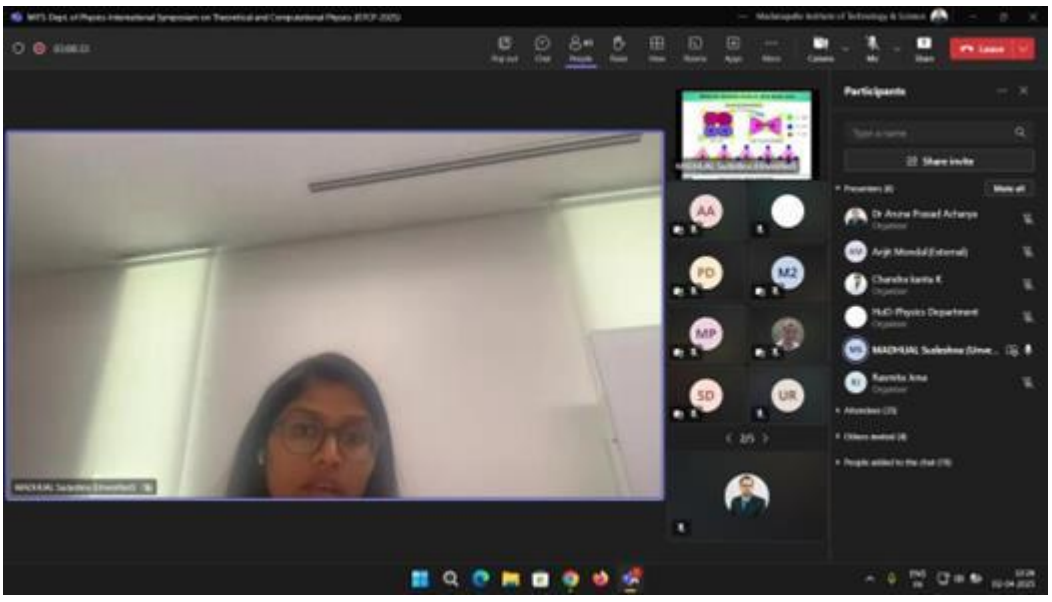
- **10:00 AM – 10:45 AM**: The sixth talk of the symposium was delivered by **Dr. Soumyaranjan Dash** from the **University of Hawaii, USA**, on the topic *"Theoretical Modeling in Solar Physics."* Dr. Dash presented an insightful discussion on how observational data can be effectively integrated into solar dynamo models to predict the evolution of magnetic fields on the Sun. His work emphasized the critical role of theoretical frameworks in enhancing our understanding of solar activity and its broader implications for space weather and astrophysical phenomena.



- **11:00 AM – 11:45 AM**: The seventh talk was presented by **Dr. Arijit Mondal** from **MITS, India**, on the topic *"Anomalies of Supercooled Water."* Dr. Mondal explored the intriguing thermodynamic behavior of water in its supercooled state, using the potential energy landscape formalism as a theoretical framework. His talk provided deep insights into the underlying mechanisms responsible for water's anomalous properties, offering a fresh perspective on one of the most studied yet mysterious substances in nature.

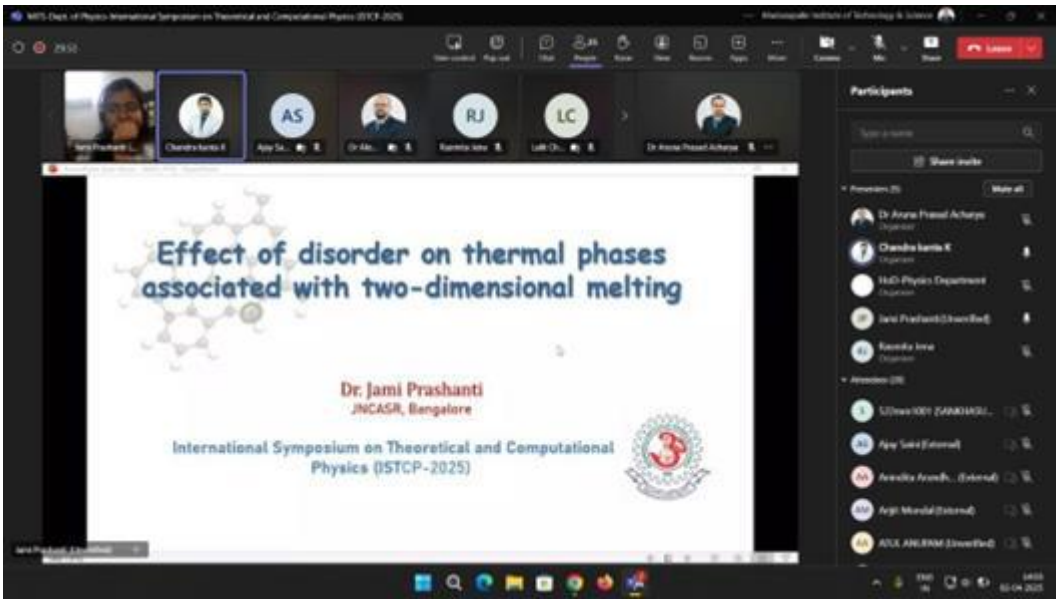


- **12:00 PM – 12:45 PM**: The eighth talk was presented by **Dr. Sudeshna Madhual** from **NIMS, Japan**, on the topic *"Ion Transport in Solid Oxide Fuel Cells (SOFCs) via MD Simulations."* Dr. Madhual utilized molecular dynamics simulations to uncover the atomic-scale mechanisms that govern ion transport in SOFCs. Her findings provided a deeper understanding of how these mechanisms contribute to improving the efficiency and performance of fuel cells, offering promising directions for future energy applications.

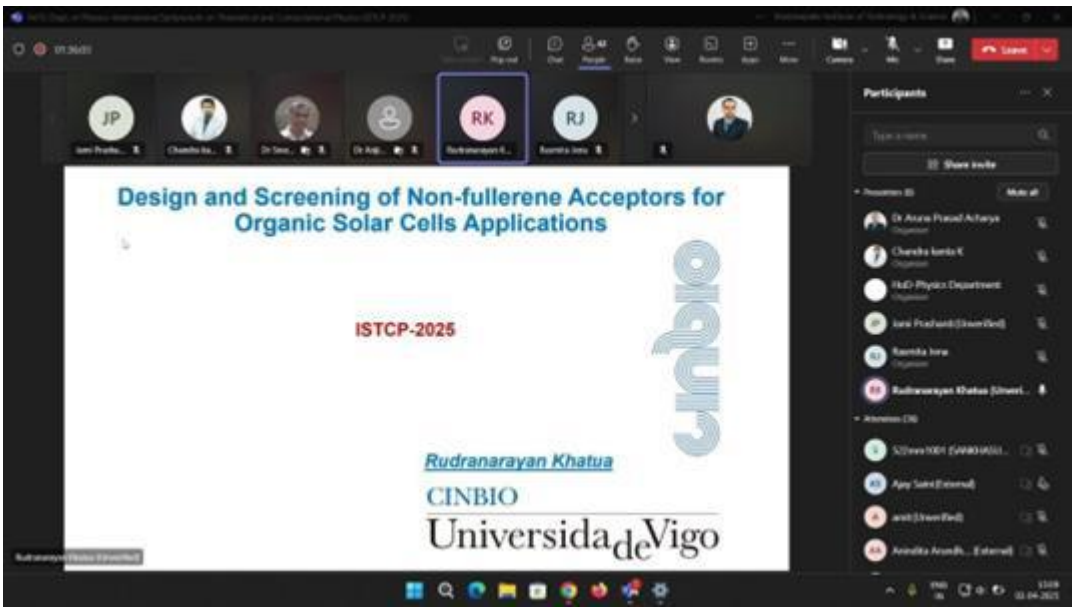


Session 4 (Session Chair: Dr. Rasmita Jena)

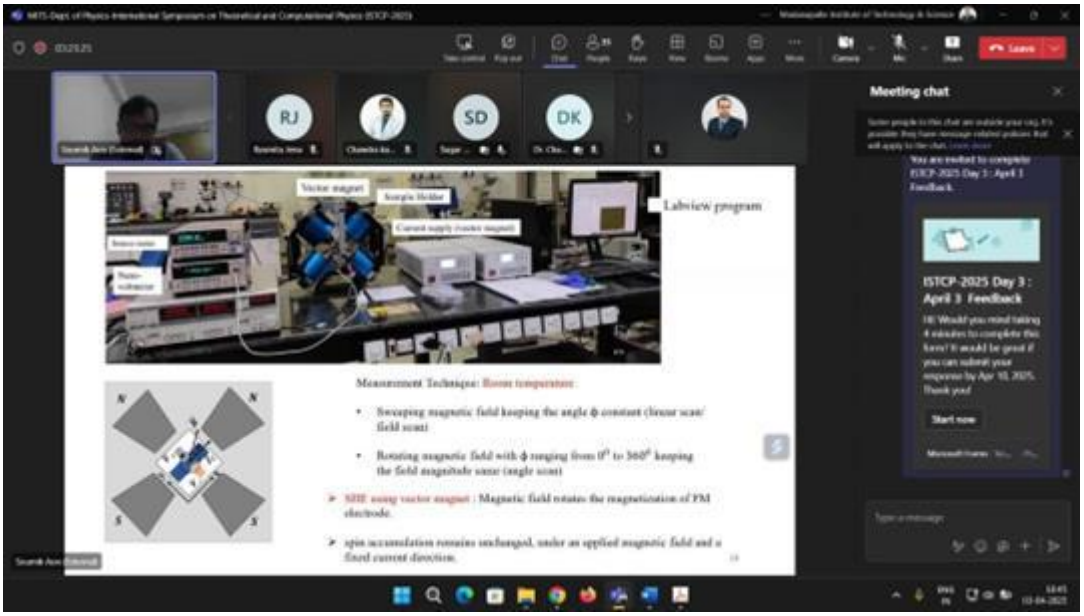
- **2:00 PM – 2:45 PM**: The ninth talk was delivered by **Dr. Jami Prashanti** from **JNCASR, India**, on the topic *"Disorder Effects on 2D Melting."* Dr. Prashanti discussed how the presence of disorder influences phase transitions in two-dimensional systems. Through a detailed theoretical analysis, she demonstrated the ways in which disorder can alter melting behavior, providing key insights into the complex interplay between structural irregularities and phase stability in low-dimensional materials.



- **3:00 PM – 3:45 PM**: The tenth talk was delivered by **Dr. Rudranarayan Khatua** from the **University of Vigo, Spain**, on the topic *"Non-Fullerene Acceptors for Organic Solar Cells."* Dr. Khatua presented an innovative approach combining density functional theory (DFT) with machine learning techniques to design and optimize high-efficiency photovoltaic materials. His talk highlighted how this integrated framework accelerates the discovery of next-generation non- fullerene acceptors, paving the way for more efficient and sustainable solar energy solutions.



- **4:00 PM – 4:45 PM**: The eleventh talk was delivered by **Dr. Aruna Prasad Acharya** from **MITS, India**, on the topic *"Non-Hermitian Delocalization-Localization Transition."* Dr. Acharya explored disorder-induced transitions in non-Hermitian quantum systems, focusing on how non- Hermiticity alters conventional localization behavior. His presentation offered key theoretical insights into the mechanisms governing these transitions, contributing to a deeper understanding of complex quantum systems beyond the Hermitian framework.



Poster Presentations (15 minutes each)

Oral Presentation Session (Session Chair: Dr. Rasmita Jena)

This session featured a diverse range of cutting-edge research topics presented by both early-career researchers and seasoned scientists:

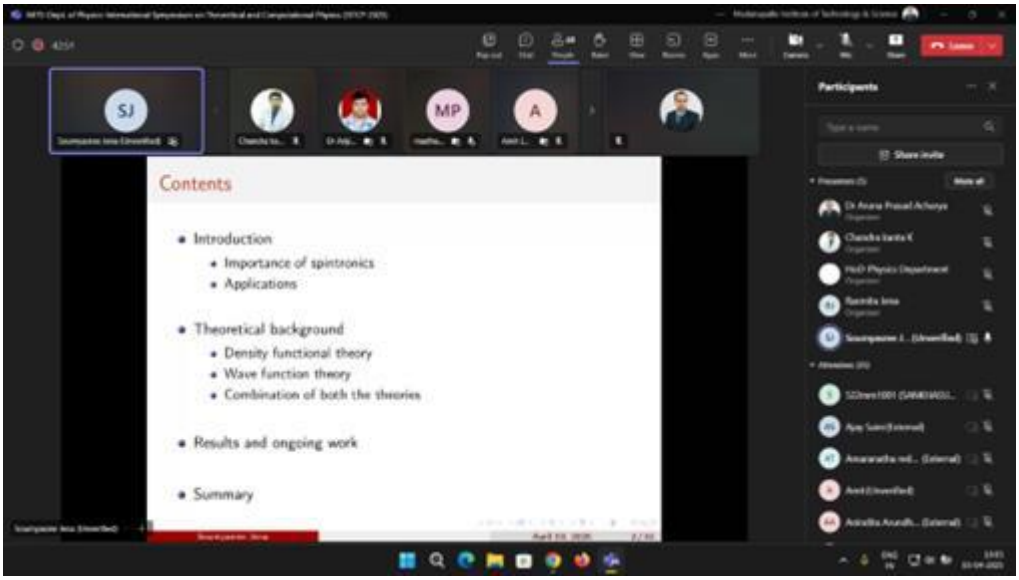
1. **Dr. Biplob Sarkar** presented *"AstroSat Observations of the Atoll Source GX S+S: A Spectro-Temporal Analysis,"* offering detailed insights into the timing and spectral behavior of the GX 9+9 system, utilizing multi-instrument data from India's AstroSat mission.
2. **Mr. Jena Akash Kumar Satrughna** shared his work on *"Unveiling the Effects of Various Aqueous Electrolytes on $NaFe(SO_4)_2$ Cathode Material for Sodium-Ion Batteries,"* focusing on how electrolyte composition influences electrochemical performance.
3. **Dr. Nithu Ashok** discussed *"Exotic Decay Modes of Og Isotopes,"* exploring theoretical predictions for the decay mechanisms of superheavy elements, particularly Oganesson, and their implications for nuclear stability.
4. **Mr. Sudipta Dash** presented *"Comprehensive Investigations of Structural, Electronic, Optical, and Thermodynamic Properties of $GeSnO_3$,"* highlighting first-principles studies that revealed the material's multifunctional potential.
5. **Dr. V. Nirupama** concluded the session with her presentation on *"Optimization of Sputtered Molybdenum Oxide Films for Gas Sensitivity,"* focusing on thin-film engineering strategies to enhance sensor performance for various gaseous analytes.

This session showcased the interdisciplinary nature of current research efforts, bridging astrophysics, energy storage, nuclear theory, materials science, and sensor technology.

Day 3 (3rd April 2025)

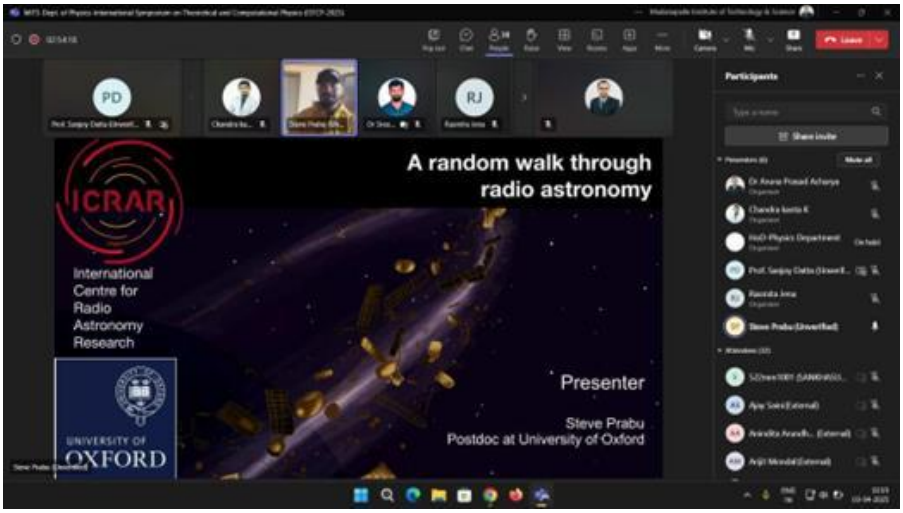
Session 5 (Session Chair: Dr. Aruna Prasad Acharya)

- **10:00 AM – 10:45 AM**: The twelfth talk was delivered by **Dr. Soumyasree Jena** from **IIT Madras, India**, on the topic *"Computational Spintronics."* Dr. Jena focused on the application of density functional theory (DFT) in the design and analysis of spin-based electronic devices. Her presentation emphasized the role of first-principles simulations in advancing spintronics, offering valuable insights into the development of next-generation technologies leveraging electron spin for information processing.



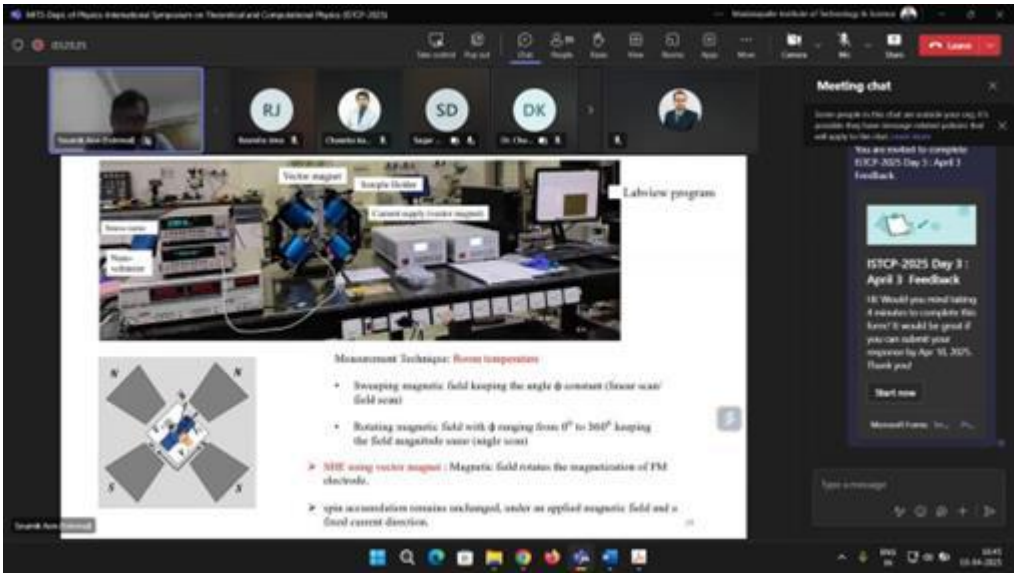
- **11:00 AM – 11:45 AM**: The thirteenth talk was presented by **Dr. Sanjoy Datta** from **NIT Rourkela, India**, on the topic *"Rashba Splitting & Altermagnets."* Dr. Datta introduced altermagnets as an emerging class of spintronic materials, distinct in their symmetry and magnetic properties. He discussed the role of Rashba splitting in these systems and highlighted their potential applications in spin-based electronics, marking a promising direction for future spintronic device development.

- **12:00 PM – 12:45 PM**: The fourteenth talk was delivered by **Dr. Steve Prabu** from **Curtin University, Australia**, on the topic *"A Random Walk Through Radio Astronomy."* Dr. Prabu took the audience on an engaging journey through the evolution of radio astronomy, tracing its progress from early radio telescopes to modern-day giants like **MeerKAT** and the upcoming **Square Kilometre Array (SKA)**. His talk highlighted key technological milestones and their impact on our understanding of the universe, offering a broad perspective on the field's past, present, and exciting future.



Session 6 (Session Chair: Dr. Rasmita Jena)

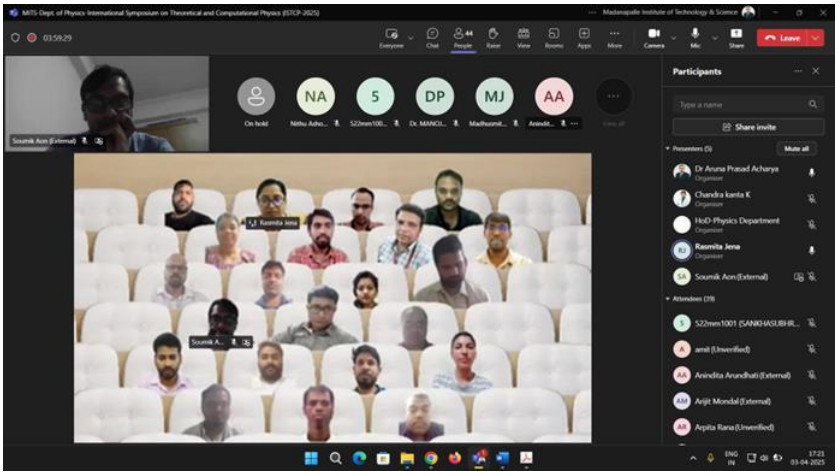
- **2:00 PM – 2:45 PM**: The fifteenth talk was presented by **Dr. Sahil Dani** from **JNCASR, India**, on the topic *"Mott Insulators in Ruthenates."* Dr. Dani explored the role of strong electronic correlations in double perovskite ruthenates, shedding light on their insulating behavior despite partially filled bands. His discussion provided valuable insights into the physics of Mott insulators and their relevance in designing materials with novel electronic and magnetic properties.
- **3:00 PM – 3:45 PM**: The sixteenth talk was delivered by **Dr. Abhisek Mohapatra** from the **University of Cape Town, South Africa**, on the topic *"Galaxy Evolution with MeerKAT."* Dr. Mohapatra showcased how deep surveys using the **MeerKAT** radio telescope are advancing our understanding of galaxy evolution by probing neutral hydrogen (HI) gas in distant galaxies. His presentation highlighted the telescope's capabilities in capturing the large-scale structure of the universe and unraveling the role of HI gas in the formation and transformation of galaxies over cosmic time.
- **14:00 PM – 4:45 PM**: The seventeenth and final talk was delivered by **Dr. Soumik Aon** from the **National University of Singapore, Singapore**, on the topic *"Spin Transport in Ferromagnetic/Heavy Metal Bilayers."* Dr. Aon presented experimental insights into spin transport phenomena, with a particular focus on magneto-impedance effects observed in doped manganites. His talk highlighted the intricate interplay between spin currents and material interfaces, underscoring the potential of these systems in next-generation spintronic applications.



Valedictory Session:

The symposium concluded with a heartfelt valedictory ceremony that encapsulated the spirit of scientific collaboration and exploration. The session began at 5:00 PM with **Dr. Rasmita Jena** delivering the opening remarks, reflecting on the enriching discussions held over the past three days and setting a thoughtful tone for the conclusion. At 5:03 PM, **Dr. Aruna Prasad Acharya** offered a warm address, emphasizing the critical role of theoretical and computational approaches in shaping the future of physics. Following this, at 5:06 PM, **Dr. M. Chandra Sekhar**, Head of the Department of Physics, delivered an inspirational message, declaring the best poster award, reiterating MITS's dedication to research excellence and academic growth highlighted the value of interdisciplinary research and its power to drive innovation and progress. Finally, at 5:10 PM, **Dr. K. Chandrakanta** delivered the vote of thanks, expressing sincere gratitude to all the speakers, participants, organizing team, and supporters who contributed to the grand success of ISTCP-2025.

Best Poster Award:



Mr. Jena Akash Kumar Satrughna from **IIT Indore** was honored with the **Best Poster Award** in recognition of his outstanding presentation and significant scientific contribution. His work, which explored the effects of various aqueous electrolytes on $NaFe(SO_4)_2$ cathode materials for sodium-ion batteries, was commended for its clarity, innovation, and potential impact on energy storage technologies.

Key Outcomes:

The International Symposium on Theoretical and Computational Physics (ISTCP-2025) proved to be a highly enriching platform aimed at fostering collaboration, knowledge sharing, and innovation across a wide spectrum of physics research. The primary objective of the symposium was to bring together leading experts, early-career researchers, and academicians working in areas such as condensed matter physics, astrophysics, nuclear physics, quantum systems, and materials science, with a strong emphasis on theoretical models, computational techniques, and high-performance simulations.

With over 60 + participants, the symposium created an engaging environment where researchers could showcase their work, gain visibility, and receive valuable feedback from established experts in their respective fields. This dynamic interaction not only helped researchers **refine their ideas** but also inspired **new directions** for future investigations through collaborative discussions.

A key outcome of the conference was the **exchange of cutting-edge research ideas** that advanced our understanding of complex physical systems—from the quantum behavior of matter under extreme conditions to the macroscopic evolution of galaxies. Sessions on **non-Hermitian quantum systems**, **spin transport**, **Mott insulators**, and **supercooled water** introduced new theoretical insights and computational tools that can influence future experimental studies. The detailed discussions on **DFT**, **molecular dynamics**, and **machine learning** in material science highlighted the interdisciplinary nature of modern physics and its application in real-world technologies like **sensors**, **batteries**, and **solar cells**.

Furthermore, the symposium played a critical role in **encouraging young researchers** by providing them a platform to present their work, receive feedback from experts, and engage in intellectual exchange. The **Best Poster Award** recognized exceptional contributions, reinforcing the importance of early-stage research and effective science communication.

For the broader scientific community, the conference served as a hub for **collaborative networking**, paving the way for future joint research projects, institutional partnerships, and student exchanges. It also provided valuable exposure to **state-of-the-art facilities** like MeerKAT, SKA, AstroSat, and advanced simulation tools, inspiring participants to adopt and apply these resources in their own work.

In essence, ISTCP-2025 significantly contributed to the ongoing development of theoretical and computational physics by **building bridges between disciplines**, **integrating theory with experiments**, and **training the next generation of physicists** to tackle the fundamental questions of science using both analytical and computational approaches.

Highlights of International Speakers

Speaker	Affiliation	Key Contribution
Dr. Divya Pandey	**University of Tartu, Estonia**	**Bridged observational techniques with galaxy evolution studies.**
Dr. Md Ramiz Aktar	**NTHU, Taiwan**	**Linked MAD-state simulations to EHT observations of black holes.**
Dr. Avinanda Chakraborty	**INAF, Italy**	**Pioneered SZ-effect studies of quasar feedback with ALMA.**
Dr. Soumyaranjan Dash	**University of Hawaii, USA**	**Advanced solar dynamo models using data assimilation.**
Dr. Sudeshna Madhual	NIMS, Japan	Decoded ion transport in SOFCs via molecular dynamics.

Dr. Rudranarayan Khatua	University of Vigo, Spain	Designed non-fullerene acceptors using computational screening.
Dr. Steve Prabu	Curtin University, Australia	Traced radio astronomy's evolution toward SKA-era discoveries.
Dr. Abhisek Mohapatra	University of Cape Town, SA	Explored galaxy evolution via MeerKAT's HI surveys.
Dr. Soumik Aon	NUS, Singapore	Innovated spintronic materials through magneto- impedance studies.

This report underscores MITS's growing role in facilitating global scientific dialogue.

SDG Mapping for ISTCP-2025

Speaker	**Talk Title**	**Relevant SDGs**	**Justification**
Dr Shreyansh Shankar Dave	Simulating evolution of energy density fluctuations in QCD plasma	**SDG G**	Advances theoretical modeling in high-energy physics, contributing to innovation in simulation tools.
Dr Divya Pandey	Introduction to Observational Astrophysics	**SDG 4, SDG G**	Promotes scientific education and innovation in astronomical observation.
Dr Md Ramiz Aktar	Simulation studies of highly magnetized accretion flows around black holes	**SDG 4, SDG G**	Enhances understanding of astrophysical systems via high-performance computing.
Dr Usuf Rahaman	Application of RMF in transitional nuclei: Os and Hg	**SDG G**	Supports research infrastructure in nuclear modeling.
Dr Avinanda Chakraborty	Quasar Feedback and SZ Signals with ALMA	**SDG G, SDG 13**	Promotes use of advanced observatories and can inform large-scale structure and energy feedback mechanisms.
Dr Soumyaranjan Dash	Theoretical modelling in solar physics assisted by observations	**SDG G, SDG 13**	Relevant to solar phenomena and can influence renewable energy research.
Dr Arijit Mondal	Anomalies of Supercooled Water	**SDG G**	Contributes to fundamental understanding in statistical physics and materials.
Dr Sudeshna Madhual	Ion Transport in Solid Oxide Fuel Cells	**SDG 7, SDG G, SDG 13**	Directly linked to clean energy technologies and innovation.
Dr Jami Prashanti	Effect of Disorders On Two-Dimensional Melting	**SDG G**	Supports development of materials modeling.
Dr Rudranarayan Khatua	Organic Solar Cell Applications	**SDG 7, SDG G, SDG 13**	Promotes clean energy through materials innovation.

Dr Aruna Prasad Acharya	Non-Hermitian De- localization to localization (DL) transition	**SDG G**	Fundamental research in quantum matter and computational theory.
Dr Soumyasree Jena	Computational Tools in Spintronics	**SDG G**	Encourages innovation in electronics and computation.
Dr Sanjoy Datta	Rashba Spin Splitting and Altermagnets	**SDG G**	Focus on advanced magnetic materials for future technologies.
Dr Steve Prabu	A Random Walk Through Radio Astronomy	**SDG 4, SDG G**	Promotes education and use of large-scale radio observation infrastructure.
Dr Sahil Dani	Mott insulating behaviour in double perovskite Ruthenates	**SDG G**	Advances condensed matter research and materials understanding.
Dr Abhisek Mohapatra	Unraveling Galaxy Evolution with MeerKAT	**SDG G, SDG 17**	Involves international collaboration and research infrastructure.
Dr Soumik Aon	Spin transport in FM/HM bilayers	**SDG G**	Supports innovation in spintronics and magnetism-based tech.

Summary of Most Relevant SDGs for the Symposium

SDG	**Description**
SDG 4	**Quality Education** – Promoting scientific literacy and training through symposium participation.
SDG 7	**Affordable and Clean Energy** – Talks on solar cells and fuel cells directly support this goal.
SDG G	**Industry, Innovation and Infrastructure** – Core SDG for your symposium focuses on research, simulation, and computational physics.
SDG 13	**Climate Action** – Applicable to solar physics, energy technologies, and environmental modeling.
SDG 17	**Partnerships for the Goals** – The international and interdisciplinary nature of the event contributes here.

Conclusion:

ISTCP-2025 successfully bridged theoretical insights with computational advancements, fostering a global research community. The symposium's outcomes will catalyze future collaborations and inspire innovative solutions in physics.