

MONDAY

COLLOQUIUM

A Playbook of Molecular Simulation, Artificial Intelligence and Experiment

Jagannath Mondal (TIFR, Hyderabad)

24 Nov 2025 (Monday) | 16:00 Hrs (Tea / Coffee 15:45 Hrs) | Venue: TIFRH Auditorium

In this seminar, I will highlight our group's foray at the interface of (bio)molecular simulations and machine learning and our attempts to interpret and integrate experiments in multiple collaborative efforts. We will initiate the seminar with case studies where biomolecular simulation was integrated with experimental observations towards data-informed model. Next, the seminar will focus on our use of artificial intelligence to discover optimised collective variables that enhance sampling and provide mechanistic insights, along with key spin-off applications involving efficient storage of trajectories and delineating patterns inherent in bacterial genome. Finally, I will discuss our recent attempts in molecular simulation and generative artificial intelligence frameworks to design novel protein sequence with tailored functions and validation via follow-up experiments.