S N BOSE NATIONAL CENTRE
FOR BASIC SCIENCES
Block JD, Sector III, Salt Lake, Kolkata 700 106

DEPARTMENTAL SEMINAR
Chemical and Biological Sciences

13th August,2024 **4.00 PM** **ONLINE / FERMION**

SPEAKER

Dr. Neelanjana Sengupta,
Associate Professor, IISER - Kolkata

Short bio :

Dr. Neelanjana Sengupta is currently an Associate Professor at IISER Kolkata since 2016. She received her PhD from the University of California, Irvine in Chemical and Materials Physics (2008). Until 2016, she worked as a Scientist at the CSIR-National Chemical Lab, Pune. At IISER Kolkata, she heads an interdisciplinary research group that uses advanced in silico approaches to probe, understand, and predict emergent phenomena in complex biomolecular systems.

Dr. Sengupta is the recipient of the CSIR-Raman Research Fellowship (2015); the Alexander von Humboldt Fellowship (Senior Researcher Category, 2020-present); and the Carl Friedrich von Siemens Fellowship (2020-present); and a bronze medal from the Chemical Research Society of India (CRSI 2024). She currently serves as the Indian Ambassador to the Biophysical Society (USA), and as the Secretary of the Indian Biophysical Society (IBS). She was one of the women scientists recognized by Vigyan Prasar (DST) in their "Future Hopes" publication (2023).

TITLE OF THE TALK

Capturing Biomolecular Responses In Silico: Opportunities and (Some) Limitations

ABSTRACT

Proteins, the machineries of life, are complex biomolecular entities whose structural, functional and thermo-kinetic behavioural patterns remain elusive despite major technological advances. Further, their response to deviant conditions, with wide relevance from therapeutics and food preservation to astrobiology, are even more challenging to characterize. In recent years, we have attempted to leverage the atomistic resolution of computer simulations to understand protein responses to non-physiological effects, arising from either one, or a combination of alterations in temperature, pressure, crowding and spatial confinement. This talk will discuss some of our evaluations for putative protein states, including folding, self-assembling and aggregating entities. Interestingly, we increasingly discover the ability of simulations to reveal surprising phenomena, such as the plausibility of self-thermophoresis. Time permitting, our efforts towards building efficient machine learning algorithms to scale biomolecular free energy barriers, will be discussed.