



**S N BOSE NATIONAL CENTRE  
FOR BASIC SCIENCES**

*Block JD, Sector III, Salt Lake, Kolkata 700 106*

## **DEPARTMENTAL SEMINAR**

# **Physics of Complex Systems**

**30<sup>th</sup> September, 2022**

**4.00 PM**

**ONLINE / FERMION**

### **SPEAKER**



**Dr. SUMANTA KUNDU,**  
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### **TITLE OF THE TALK**

## **Machine learning predictions of complex polymer topologies**

### **ABSTRACT**

From tying shoelaces to maneuvers in sailing or mountaineering, knots are useful in our everyday lives. At microscopic scales, knots have been shown to occur naturally in DNA, proteins, and more generally, in long polymer chains. Identifying the topology of a knotted structure is a fundamental challenge in the field of polymer physics as the cell functionalities and biological responses are mediated by the topological complexity. In this talk, I will present a brief overview on knots and discuss the usefulness of machine learning techniques in polymer physics.

By employing deep learning approaches, we investigate the ability of neural networks (NN) to accurately classify the topology of different knotted polymers. We find that the performance of NN is reasonably well even for polymer chain lengths and densities other than the trained ones. The NN is also able to learn the knot families (torus/twist knots). Moreover, we show that the NN eases out the complexity involved in studying the topological relaxation dynamics for open polymer chains

### **HOST FACULTY**

**Prof. Punyabrata Pradhan and Prof. S. S. Manna**

**DEPT. OF PHYSICS OF COMPLEX SYSTEMS**

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