

# Applied Physics & Machine Learning Seminar Series, IIT Hyderabad

Online webinar on **Oct 06, 2020 at 2:30 PM**



भारतीय प्रौद्योगिकी संस्थान हैदराबाद  
Indian Institute of Technology Hyderabad

Date : 06-10-2020  
Time : 2:30 PM (IST)  
Topic : Seminar at IITH  
Speaker : **Dr. Arghya Dutta**  
Affiliation : Max Planck Institute for Polymer Research, Mainz, Germany  
Title : **Data-driven Search for Structure–Property Relations in Soft Matter**  
Link : <https://meet.google.com/mih-hojp-oyc>



## Abstract

Connecting a material's structure and easily measurable properties to a different property that is of practical interest but hard to measure is of fundamental importance in soft matter systems. Data mining—the process of finding associations, correlations, and anomalies in data—can significantly facilitate the search for finding these generalized structure-property relationships. In this talk, I will describe two problems where we have used data mining to relate structure to property. In the first part, I will describe how data-driven methods can be successfully used to discover a recurring structural motif in self-assembling peptides that can heal damaged neurons. In the second part, I will talk about our ongoing search for key physical descriptors that correlate with the passive permeability of a drug molecule across lipid bilayer to expedite drug discovery. Finally, I will outline how we can employ our data-driven methods in biomaterials to discover structure–property relations.