**Tata Institute of Fundamental Research**
Survey No. 36/P, Gopanpally Village, Serilingampally, Ranga Reddy Dist., Hyderabad - 500107

# Students' Annual Seminar

## Applications of Machine Learning for Bio-molecular Simulations

## Satyabrata Bandyopadhyay

Machine Learning has emerged very promising techniques nowadays. After the advancement of these methods, it is finding a lot of applications; almost everywhere in Science and Technology. In this talk, I will show how Machine Learning especially Deep Learning techniques can be successfully applied for Bio-molecular Simulations. Here, we have employed deep learning techniques for protein folding simulations and have identified potentially good collective variables or order parameters in hidden dimensions. Along the hidden dimensions we have characterized both qualitatively and quantitatively the relevant meta-stable states for folding of some peptides and mini-proteins.

***Monday, Feb 24th 2020***

***10:30 AM (Tea/Coffee at 10:15 AM)***

***Seminar Hall, TIFR-H***