



## Institute Colloquium



5 April, 2022



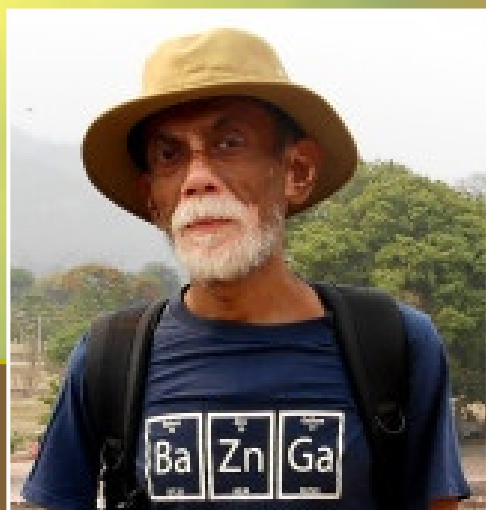
4.00 PM



Webinar Link



YouTube Link



### Title:

**Minor conformation-triggered intermolecular interactions**

### Abstract:

Many molecules display a distribution of multiple conformations where the population of one conformation dominates. However, when these molecules interact with another molecule, such as in protein-protein, DNA-protein or DNA-ligand interactions, often there is a population shift in the conformational ensemble a minor conformation becomes the dominant interacting conformation. Such a shift can occur via two limiting mechanisms. In the 'conformational selection' model, an otherwise unstable but pre-existing conformation is the conformation that facilitates binding and thus becomes the dominant conformation post-binding. In the 'induced fit' model, binding is triggered by the pre-existing major conformation but it undergoes a conformational change upon binding, where the final bound conformation could either be a pre-existing minor conformation or a new conformation that did not exist prior to binding.

In this talk I will discuss some recent results from my research group where we experimentally probed population shifts in the conformational ensemble of a molecule after it interacts/binds with a partner molecule. The first example will cover binding of a designed DNA-binding NIR fluorescent probe. The second example will cover the mechanism that facilitates phosphorylation of a buried serine residue in the bacterial toxin protein HipA. We show that DNA minor groove induces *acis-trans* isomerization in the ligand it binds. For HipA we could identify a minor conformation where the buried serine residue is exposed a conformation compatible with facile phosphorylation. Both the examples show how minor conformations can play an important role in intermolecular interactions. Implications for our results will be discussed including a detailed analysis of 'conformational selection' versus 'induced fit' model for the ligand-DNA interaction.

### Speaker:

**Professor Gautam Basu**  
Department of Biophysics  
Bose Institute, Kolkata