

SEMINAR

Department of Biological Sciences



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Hosted by Professor Prakash Kumar



The Shapes and Structures of Biomolecules

Computational Models and Biological Insights

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The molecular basis of life rests on the activity of biological macromolecules, mostly nucleic acids and proteins. A perhaps surprising finding that crystallized over the last handful of decades is that geometric reasoning plays a major role in our attempt to understand these activities. The shape of a protein for example defines its function, as it determines what substrates it can interact with. It is also noteworthy that protein geometry is not rigid: small changes in the shape of a protein can have a large effects on its behavior. In this seminar, I will explore the relationships between the geometry, dynamics and function of a biomolecules. I will cover two topics: (1) I will look at the influence of the environment (solvent and ionic atmosphere) on protein shape and function, using an ion channel to illustrate insights gained from simple models, and (2) I will describe new methods for sampling the conformational space between two instances for the structure of a bio-molecule as well as illustrate how the same techniques can be applied to study the geometry of evolution.