



**TIFR Centre for Interdisciplinary Sciences,  
Narsingi, Hyderabad 500075**

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## **Seminar**

### **Simulating at Multiple Scales: Application to Chemistry and Biophysics**

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The chemical and biological processes are complex and intriguing in nature. Understanding the mechanisms and implications of these processes requires consideration of the aspect of diverse length and time scales associated with them. In this respect, computer simulation is gaining attention as one of the promising tools. In this presentation, I will highlight certain problems of chemical and biophysical relevance, which I have addressed using computer simulation at different scales. The problems will involve visiting the kinetics of ligand-protein binding at nano-scale, looking at collective behavior of peptide-membrane interaction at an intermediate scale and understanding self-assembly of materials at a large scale. One of the purposes of this talk will be rationalizing the usage of models at different resolution and different simulation techniques to access the diverse spatial and temporal aspects inherent in those problems. The mechanistic insights learnt from the simulations will be discussed and will be compared against relevant experimental inputs. Finally, future directions will be briefly discussed.

***Saturday, Dec 21<sup>st</sup> 2013***

***11:30 AM (Tea/Coffee at 11:15 AM)***

***Seminar Hall, TCIS***