**Tata Institute of Fundamental Research**
Survey No. 36/P, Gopanpally Village, Serilingampally, Ranga Reddy Dist., Hyderabad – 500 046

# Seminar

## Non-equilibrium Modelling of Solution Crystallisation using Constant Chemical Potential Molecular Dynamics Simulations

## Tarak Karmakar

### IIT, Delhi

In my talk, I will be discussing a new non-equilibrium simulation method, Constant Chemical Potential Molecular Dynamics (CmuMD), and its applications in modelling concentration-driven processes such as solution crystallisation. During crystallisation, solute molecules are continuously drawn from the solution to the growing crystal, and a closed finite-size system fails to maintain a constant thermodynamic driving force for crystallisation - the solution supersaturation. Such solution depletion affects the further growth of the crystal. The CmuMD method helps in maintaining constant solution concentration near a growing crystal slab or a nucleus and thereby mimics a realistic solution crystallisation process. Besides successful modelling of realistic crystallisation processes, this method and its variants find applications in simulating other concentration-drive processes such as adsorption (electrochemical) and separation of gas and liquids across membranes.

***Friday, July 8th 2022***

***04:00 PM***

***Auditorium***