Tata Institute of Fundamental Research
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Internal Webinar

Macromolecular crowding effects in crowded biomolecular environments

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High concentrations (300-400 g/l) of different biomolecules (proteins, nucleic acids, metabolites) in "crowded" biological environment impede the accuracy of various experimental and computer simulation studies. Computer simulation approaches like: rigid-body Brownian dynamics, Monte Carlo simulations are promising alternatives for studying macromolecular crowding at a microscopic level. In this presentation, I will discuss the impact of macromolecular crowding on protein-protein interactions, relative stabilizations and destabilizations of flexible polymer conformations in self crowding conditions and in presence of protein crowders. For this purpose, a **multiple conformation Monte Carlo (mcMC)** simulation approach has been employed. Protein-protein interaction has been studied for Hen egg white Lysozyme (HEWL) solutions at different ionic strengths. Further, flexible polyethylene glycol (PEG) polymers were studied in self crowding as well as in presence of protein crowders to study competition of excluded volume effect and nonspecific interactions.

Thursday, Jun 18th 2020

10:30 AM