Tata Institute of Fundamental Research
Survey No. 36/P, Gopanpally Village, Serilingampally, Ranga Reddy Dist., Hyderabad - 500107

Seminar

Molecular Scale Spatiotemporal Organization in Biological membranes: Insights from nonaffine displacements

Anand Srivastava

IISc, Bangalore

The rich structural complexity of biological membranes arises from the chemical diversity of its constituents. Differential inter and intra-molecular interactions result in preferential segregation and clustering of certain types of lipids and proteins, giving rise to a variety of lateral organization on the membrane surface. We analyze multiple long timescales (tens of microseconds long) all-atom molecular dynamics simulation trajectories with carefully chosen lipid compositions that reproduce a variety of phases. We numerically calculate the non-affine displacements (x^2) of individual lipids in their local neighborhood and use this framework to get deeper insights into the spatiotemporal nanoscale organization in biological membranes. In this talk, I will use this new framework for membrane analysis to discuss the following findings and ongoing work: (i) We find that x^2 works as a high-fidelity marker between the liquid order (L_o) and liquid disordered (L_d) regions in the membrane system at molecular length scales (ii) We find that distributions in x^2 and lipid packing defects are strongly correlated and the correlations reveals some interesting molecular-level insights that may be useful in understanding preferential localization of certain peptides and proteins at fluid-phase boundaries. In this part of the presentation, I will also discuss our work on interpretation of phase boundary fluctuation spectra on interfaces with and without inclusions (peptides) (iii) Lastly, a central question we are trying to address is the possibility of degeneracy in membrane organization at nanoscales using ideas from energy landscape theory and Statistical Mechanics based optimization process and the x^2 distribution framework. We use the MD trajectories of coexisting fluid-phase bilayer systems to develop a continuous lattice Hamiltonian and we evolve that using Monte Carlo simulated annealing algorithm to explore the possibility of structural degeneracy in membrane organization. We show that lipids with more bio-mimetic characteristics are capable of having degenerate nanoscale structures on membrane and the local patterns (in terms of phase organization) could be pathway/environment dependent. We argue that the biological lipids with physiological constitution have a frustrated energy landscape with multiple equivalent valleys with respect to the localized molecular-scale membrane organization and this structural degeneracy at the nanoscale could provide for a larger repository to functionally important molecular organization ("functional nanodomains"). Time permitting, I will also discuss how we are using this framework to draw parallels between dynamics in glassy systems and lipids in liquid ordered phase and understand the molecular-origin behind the dynamical heterogeneity in the biological membranes.

Tuesday, Aug 13th 2019

4:00 PM (Tea/Coffee at 3:30 PM)

Auditorium, TIFR-H