Department of Chemical Engineering, IIT Hyderabad
Scientific Seminar Series 2026

Date: 10-04-2026
Time: 02:30 PM (IST)
Speaker: Prof. K. Ganapathy Ayappa
Affiliation: Chemical Engineering, IISc Bangalore
Title: Unravelling molecular interactions with the bacterial cell envelope
Venue: LHC-03

Abstract

With rising bacterial resistance, there is a pressing need to develop a molecular understanding of the interactions of antimicrobial molecules with the complex topology of the bacterial cell envelope. Using molecular dynamics simulations at different time and length scales, we are able to probe a wide variety of phenomena ranging from a few nanoseconds to several microseconds. In this talk, I will summarize our ongoing efforts aimed at understanding the barrier properties of bacterial cell envelopes and the challenges involved in studying Gram positive and Gram-negative bacterial strains. We develop molecular models at both atomistic and coarse-grained scales for different layers of the cell envelope and assess several structural and mechanical properties, as well as the insertion free energies of small molecules. Barrier properties are reconciled with diffusion coefficients measured using fluorescence correlation spectroscopy. Lastly, I will talk about recent work where we use coarse-grained simulation data to develop kinetic models to quantify the partitioning of preservative molecules and surfactants with the bacterial membrane. Novel first- and zeroth-order membrane partitioning kinetics are observed, and models developed to rationalize these two distinct kinetic regimes will be discussed. Our molecular dynamics simulations can potentially open up in silico models for the screening and development of novel therapeutics against virulent bacterial infections.

Biography

Professor Ayappa obtained his Bachelors degree in Chemical Engineering from Mangalore University, India in 1984, and an MS and PhD in Chemical Engineering with a Minor in Mathematics from the Department of Chemical Engineering and Materials Science at the University of Minnesota, in 1992. Professor Ayappa has held visiting positions at the University of North Carolina, the James Franck Institute at the University of Chicago and Department of Materials at ETH Zurich. He is a fellow of the Indian National Academy of Engineers and the National Science Academy. His interests lie in developing a molecular understanding of structure and dynamics of molecules at the nanoscale using molecular simulations and statistical mechanics. Current interests lie in the area of biological membranes, membrane protein interactions implicated in bacterial and viral infections and cellular signalling and dynamics at the nanoscale.