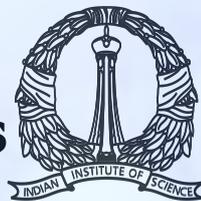


Monthly informal seminar series on Integrative Modelling in Biophysics

presented by
Molecular Biophysics Unit, IISc



Integrative Modelling Tools and Simulation Technologies for Cell-Scale Structural Biology

In parallel to advances in structural biology of SARS-CoV2, a major objective in computational studies has been to develop complete models of the virus needed for simulation studies of the virus penetration into the host cell, and to provide a structural framework for novel therapeutic strategies. Modeling such large molecular assemblies at sufficiently high detail and quality, however, poses major challenges. I will share a robust, automated protocol including advanced modeling tools combined with multi-scale MD simulations to construct optimally packed arrangements of (10,000s) lipids and (1,000s) proteins at any desired densities and in any desired shape, for example the entire SARS-CoV2 viral envelope or the endoplasmic reticulum (ER) membrane. Along with lessons learnt and solutions to challenges during the process, I will also discuss the results of the simulations performed on whole viral envelope structures.



Prof. Emad Tajkhorshid

**J. WOODLAND HASTINGS
ENDOWED CHAIR IN
BIOCHEMISTRY**

University of Illinois

**Date: 9-Aug-2022 (Tuesday)
Time: 17:30 hours (IST)**

For queries, contact:
Anand Srivastava (anand@iisc.ac.in)

Emad Tajkhorshid is Hastings Endowed Chair in Biochemistry, as well as holds additional appointments in Chemistry, Bioengineering, Pharmacology, Biophysics and Quantitative Biology, and Computational Science and Engineering. He received a Ph.D. in molecular biophysics from the Heidelberg, before moving to UIUC for his postdoctoral studies in computational biophysics. He joined the faculty of Biochemistry in 2007 and was fast tracked to associate professor in 2010 and then again to the rank of professor in 2013. His tenure dossier was selected as one of the two top UIUC tenure cases on campus. In 2015, he was named a University of Illinois Scholar, after being nominated by both UIUC and UIC campuses. In 2016, he was named Endowed Chair in Biochemistry. Dr. Tajkhorshid is a world leader in developing and applying advanced computational techniques to characterization of membrane protein function. He has authored 290 research articles (Google H-index 78) with ~37,000 citations.

Link: <http://mbu.iisc.ac.in/IMSS/index.html>