



RAKESH VAIWALA

Post-Doctoral Fellow

Chemical Engineering
Indian Institute of Science,
Bangalore



SHORT BIO

I am from Gujarat, India. I took professional trainings in chemical engineering at IISc and IIT Bombay.

My research interest is in developing molecular models for simulating bio-membranes and proteins both at atomistic as well as coarse-grained scales.

CURRENT RESEARCH

My research focus is on modelling Bacterial cell walls and lipid membranes. To investigate the membrane-protein interactions using molecular dynamics simulations is of prime interest.

CONTACT

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EDUCATION

PhD, Chemical Engineering **Indian Institute of Technology, Bombay**

Jan 2014 - July 2018

Thesis title: Physics of Bilayer Interactions and Membrane Electroporation using Mesoscopic Simulations

Thesis Advisor: Prof. Rochish Thaokar and Prof Sameer Jadhav

M. Tech, Chemical Engineering **Indian Institute of Science Bangalore**

Aug 1999 - Jan 2001

B. Tech, Chemical Engineering **[Sarvajanik College of Engineering & Technology]**

1995 - 1999

WORK EXPERIENCE AND FELLOWSHIPS

Fluent India Pvt Limited, Pune, India (Application Engineer)

Jan 2001- Sep 2002

Sarvajanik College of Engineering & Tech. Surat, India (Lecturer) [2009 - 2013]

Selected publications

Rakesh Vaiwala and Ganapathy Ayappa, *A Generic Force Field for Simulating Native Protein Structures Using Dissipative Particle Dynamics*, *Soft Matter* 17(42), 9772-9785, (2021)

Rakesh Vaiwala, Pradyumn Sharma, Mrinalini Puranik, and K. Ganapathy Ayappa, *Developing a Coarse-Grained Model for Bacterial Cell Walls: Evaluating Mechanical Properties and Free Energy Barriers*, *J. Chem. Theory Comput.* 16(8), 5369-5384, (2020)

Pradyumn Sharma, Rakesh Vaiwala, Srividhya Parthasarathi, Nivedita Patil, Morris Waskar, Janhavi Raut, Jaydeep Basu and Ganapathy Ayappa, *Interactions of surfactants with the bacterial cell wall and inner membrane: Revealing the link between aggregation and antimicrobial activity*, *Chemical Science* [In Review]