europass

Lakshmi kumar Kunche

WORK EXPERIENCE

01/04/2022 - 30/06/2023 Blacksburg, United States
POSTDOCTORAL ASSOCIATE VIRGINIA TECH

Business or Sector Education **Department**Chemical Engineering

EDUCATION AND TRAINING

14/07/2014 - 20/01/2022 Chennai, India
DOCTOR OF PHILOSOPHY Indian Institute of Technology Madras

Final grade8.21/10

04/10/2010 - 30/04/2014 Vishakhapatnam, India
BACHELOR OF TECHNOLOGY Andhra University

Final grade8.9/10

ADDITIONAL INFORMATION

PUBLICATIONS

Structure and dynamics of aqueous solutions containing poly-(acrylic acid) and non-ionic surfactant pentaethylene glycol n-octyl ether (C8E5) : A molecular simulations study
- 2021

Computational Materials Science, 2021, 186, 110043.

Structure and dynamics of an aqueous solution containing poly-(acrylic acid) and non-ionic surfactant octaethylene glycol n-decyl ether (C10E8) aggregate and their complexes investigated by molecular dynamics simulations
- 2021

Soft Matter, 2021, 17, 670-687.

Detailed molecular structure of glassy poly(phenylene oxide)(PPO) studied by molecular dynamics simulations
- 2020

Journal of Macromolcular Science, Part B: Polymer Physics, 2020, 59, 796-820.

Conformations and solvation of synthetic polymers in aqueous solution using implicit solvent molecular dynamics simulations
- 2023

Journal of Physical Chemistry B, 2023

A review of recent advances and applications of machine learning in tribology - 2023

Physical Chemistry and Chemical Physics, 2023

Data driven computational design and experimental validation of drugs for SARS-CoV-2 – 2023

Journal of Physical Chemistry Letters, 2023, 14, 9490-9499.

Atomistic insights into the solubility of α-glucans in water – 2023

Submitted to Journal of Carbohydrate Polymers

PROJECTS

Investigation of interactions between 6LU7 protein and functionalized and bare ligands using atomistic molecular dynamics simulations

- Interaction of proteins with ligands using MD simulations and drug docking
- Mechanical properties of E-coli and marine csgA proteins
- Tribological properties of polysaccharide-basedlubricants

Molecular simulation studies of uncharged and charged polymers in aqueous solution and their complexation with non-ionic and ionic surfactants · MD investigation the structure of polymer-surfactant complexes in aqueous solutions and structure of surfactant micelles in aqueous solution.
· Thermodynamics of micellization in polymer-surfactant-water ternary solution
· Structure and thermodynamics of polyelectrolytes in solution using MD simulations
· Structure and thermodynamics of uncharged polymers in aqueous solution using implicit solvent MD simulations
· Computer administrator responsible for installation and maintenance/upgrades of software, OS and maintenance of hardware for the workstations in the Macromolecular Modeling and Simulation lab

COMPUTING SKILLS AND SIMULATION METHODS

Simulations

· Atomistic and implicit solvent molecular dynamics simulations, DFT and free-energy simulations
· Coarse-grained and Mesoscale Simulations
· Drug docking on proteins
· Machine Learning and Deep Learning
· System administrator for maintaining computing nodes/Workstations (2016-2020).

SOFTWARE SKILLS AND EXPERTISE

Commercial Softwares

Gromacs, LAMMPS, Gaussian, Material studio, VMD, Packmol, Avogadro, Gaussview, Chem Window, COMSOL, Aspen, VOTCA

Languages/Softwares/OS

Python, C, C++, R, Shell scripting, Origin, GNUPLOT, Linux, Windows.

CONFERENCES AND SEMINARS

Indianapolis, USA
ACS Spring 2023, March 26-30, 2023

Udaipur India
International Conference on Functional Electroceramics and Polymers (ICEP2019)

Jaipur India
3rd International Conference on Softmatter 2018

Delavan USA
Foundations of Molecular Modeling and Simulation (FOMMS 2018)

Pune, India
SPSI-Macro 2018

Jaipur, India
International Conference on Frontiers at the Chemistry-Allied Sciences Interface (FCASI-2016)