COLLEGE OF ENGINEERING

SEMINAR ANNOUNCMENT

"Investigating Model Asphalts and Transmembrane Protein Plexin Using Molecular Dynamics Simulations"

Presenter by Dr. Liqun Zhang

Abstract

In the first part of the talk, both Monte Carlo (Towhee program) and molecular dynamics simulations (LAMMPS program) were performed on model asphalts with the goal to improve the performance of asphalt on road pavement. Asphalt is originally from crude oil distillation, and is widely used on road pavement, but its composition is poorly defined. Based on solubility and polarity, asphalt can be divided into three parts. Model asphalt mixtures were built for simulation input by choosing one to three compounds to represent each part. The microstructure of molecules inside the system, and the main physical and mechanical properties of asphalts were calculated, and the relationships among microstructure, properties and chemical compositions of asphalt were then analyzed. It was found that adding one polystyrene chain into the original model asphalt can improve its high temperature performance. In the second part of the talk, a protein, namely Plexin-B1, was investigated using both CHARMM and NAMD molecular dynamics simulations with the goal to understand its signal transduction mechanism. Plexin-B1 is a single-pass transmembrane protein, belonging to the plexin family, which play important roles in axon guidance, angiogenesis, and cancer development. Plexin can receive semaphorin guidance cues, and transfer signals through the lipid membrane. Based on microsecond long all atom molecular dynamics simulations, the transmembrane oligomer structures of Plexin-B1 were predicted. Connecting them with the intracellular domain of Plexin-B1 complexes bound with small Rho and Ras GTPases, the all atom model of plexin-B1 in both the monomer and trimer forms were set up. The structure and dynamics analysis based on molecular dynamics simulations strongly suggest that both GTPases and lipid bilayer play an important role in the functional process of Plexin-B1.

About the Speaker

Dr. Liqun Zhang is an Assistant Professor in the Department of Chemical Engineering. She earned her Ph.D. in Chemical Engineering of University of Rhode Island. After that, she worked as a postdoc initially in the Chemical Engineering and Geological Science department later in the Physiology and Biophysics department of Case Western Reserve University focusing on protein structure and dynamics using computer simulation method. Her future interest includes investigating the structure, dynamics and functions of proteins and engineering materials using molecular dynamics simulation method.

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Time: 12 P.M. – 1 P.M.
Location: Prescott 225