הטכניון - מכון טכנולוגי לישראל

TECHNION - ISRAEL INSTITUTE OF TECHNOLOGY

הפקולטה להנדסה כימית
ע"ש וולפסון
The Wolfson Department of Chemical Engineering

Wolfson Department of Chemical Engineering Seminar
Zoom seminar / Zoom ID: 97577956516

Wednesday - May 2nd 2022 at 13:30 (Israel time)

Investigation on Human β Defensin and Asphalt using Molecular Dynamics Simulation Method

Dr. Liqun Zhang
Department of Chemical Engineering
Tennessee Technological University

Human β defensin type 3 (hBD-3) is a small antimicrobial peptide. It belongs to the human innate immune system and is mainly secreted by the epithelial cells. It has microbicidal activities against both Gram-positive and Gram-negative bacteria, fungi, yeast, some enveloped virus, and even plays a role blocking covid-19 virus attacking human normal cell receptors, besides having chemotactic activities. In order to understand its functional mechanism in molecular detail, the initial binding structure of hBD-3 on model bacterial membrane was predicted using both microsecond-long molecular dynamics simulations (a computer simulation method for analyzing the physical movements of atoms and molecules) and solid-state NMR method. It was found that hBD-3 binds with bacterial membrane on the two loop regions. The contribution of each residue on hBD-3 to its binding with bacterial membrane was calculated using the free energy perturbation (FEP) method. It was found that the β2, β3 and the second loop regions mostly contribute to the binding of hBD-3 with membrane through electrostatic interactions.

The second part of this talk will focus on a different system, asphalt. Asphalt is originally from crude oil distillation, and is widely used on road pavement. Based on its solubility in different solvents, asphalt can be divided into three parts: asphaltene, resin and maltene. Model asphalt mixtures were built by choosing one to three compounds to represent each part for simulation input, which can possess several physical and mechanical properties of real asphalt but could not replace real asphalt to be used on road pavement. Based on molecular dynamics simulation trajectories, both the microstructure and major physical properties were calculated. It was found that the asphaltene molecules at high temperature could form aggregation. Viscosities of the original model asphalt mixtures have strong temperature dependence. When asphalt was modified with the model waste vegetable oil (WVO) mixture, the densities of asphalt at high temperatures increased, the packing of molecules at low temperatures became more random, the diffusion rates of components in asphalt increased, and the viscosities at low temperatures decreased. The simulation result can explain the experimental findings that implementing waste vegetable oil can improve the performance of asphalt at low temperatures.

In this talk, the same simulation methods to solve more interesting future research areas will be proposed, including biomass, bioasphalt, and hBD-3 interaction with both inner and outer layers of Gram-negative membrane and Gram-positive membrane, and with chemokine receptors.