A quick overview of computational chemistry on membrane systems

Jindřich Lněnička

Biological membranes are a vital part of every known living organism. As they present a natural barrier to both drugs and other xenobiotics, thorough understanding of interactions on the molecular level is vital for both efficacy of treatments and potential toxicity. Furthermore, artificial lipid membranes can be used as a drug carrier in forms of liposomes and lipid nanoparticles.

In order to obtain molecular level of insight, computational methods can be used as they are relatively cheap, fast and detailed. For this purpose, molecular dynamics is an especially suitable tool as it provides the whole trajectory and the detailed mechanism of the interactions.

In this presentation, the two use-cases are shown. One, where atomistic simulation is further coarse-grained to be scaled to a vesicular model to uncover the interactions of outer layer of Gram-negative bacteria membranes and sheets of graphene of various sizes and modifications. There, it was observed, that lipopolysaccharide layer is impermeable for the graphene sheets.

Second use-case is an industrial one as it shows a temperature-dependant interaction of apixaban and a liposomal model to illustrate a mechanism of liposomal formation.