

In this thesis, we start with the description of the biophysical properties of the plasma membrane models upon signaling processes such as the increased cytosolic concentration of calcium ions, or posttranslational modifications of membrane proteins. Calcium signaling is characterized by a rapid increase of its cytosolic concentration. We identify calcium binding sites and characterize the binding in the plasma membrane models of increasing complexity from pure phospholipid bilayers, through cholesterol and peptide rich lipid membranes, to membranes extracted from HEK293 cells. We use Time-Dependent Fluorescent Shift method, which provides direct information on hydration and mobility in defined regions of a lipid bilayer, accompanied with molecular dynamic (MD) simulations, which give molecular details of the studied interactions.

The initial step of signaling mediated by PAG protein is its double palmitoylation. We investigate changes of the biophysical properties of both the lipid membrane and the peptide itself upon the incorporation of the palmitoyls. Employing all atom MD simulations, we study inter- and intramolecular interactions as well as changes in membrane hydration, thickness, or lipid ordering.

The second part of the thesis, realized in a direct collaboration with a pharmacological company, is focused on the tear film (TF) of the human eye and related pharmacological issues. We use extensive coarse grain MD simulations to mimic big patches of the TF and investigate the molecular mechanism of the TF stabilization upon addition of surfactant molecules, which are being developed for the treatment of dry eye disease.