# Influence of Lipid Shape and Headgroup Charge on Bilayer Behavior

*Klemen Bohinc*[1]

[1] *Faculty of Health Sciences, University of Ljubljana, SI-1000 Ljubljana, Slovenia*

*klemen.bohinc@zf.uni-lj.si*

To better understand bilayer property dependency on lipid electrostatics lipid head group's internal degrees of freedom need to be taken into account. The most general shapes and charge distributions of lipid head groups are considered: rigid rod-like, flexible segments and triangular head groups. The lipid monolayer is in contact with an electrolyte solution composed of monovalent ions. The system is considered by means of a generalized classical Density Functional Theory model and Simulations. Starting from the free energy of the system the calculus of variation was used to derive Euler-Lagrange equations which were solved numerically by Finite element method [1-4].
Results show that there are mainly two distinct regions of the electric double layer: (1) the interfacial region, with thickness less than or equal to the length of the fully stretched conformation of the lipid head group, and (2) the outside region, which follows the usual screening of the interface. The lipid head group structure substantially impact the potential profile of the layer. The strongly charged monolayer induces a non-monotonous conditional probability density and tendency of head groups more perpendicular to the surfaces. The weakly charged surface causes more constant conditional probability density. The flexibility of head groups switches the perpendicular to more parallel orientation of head groups due to possibility of intermediate positive charge to be in the vicinity of negatively charged plane of phosphate groups and terminating negative charge to be extended more in the solution. Simulations confirm the results of the model [4].
Finally, a phase-separated multi-component phospholipid plane with one half consisting of charged lipids and the other half of non-charged lipids in contact with an electrolyte solution composed of monovalent ions will be considered. Results show that in the vicinity of the transition from the uncharged to the charged part a sigmoidal transition to an increased concentration of counterions is observed [5].

**Keywords:**
Lipid head group structure, Electric double layer, Phase separation

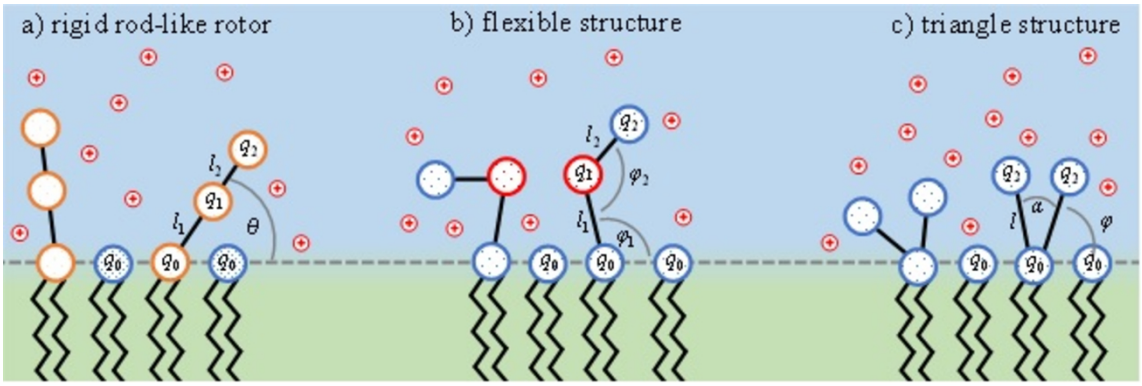


*Figure 1. Schematic presentation of the lipid monolayer, where head-groups with the spatial charge distribution are in contact with the aqueous solution [4].*

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