Abstract

At the cellular level both membrane curvature, or shape, and the electrostatics of membranes play critical roles in a wide range of processes. Lipid bilayer membranes are curved to achieve compartmentalisation of the entire cell and the organelles. Locally, this curvature is involved in processes such as protein sorting and membrane scission and fusion. Similarly, the electrostatics of membranes have significant roles to play in both signalling and passive ion transport.

In this PhD thesis, a connection between membrane curvature and membrane electrostatics is investigated. It turns out, that these two properties of the membrane, which does not seem correlated, are linked by various mechanisms. More specifically, two such effects are investigated here: 1) the so-called flexoelectric effects, and 2) the effect of local application of calcium ions to a negatively charged lipid bilayer.

The flexoelectric effect describes the relationship between mechanical deformations of the lipid bilayer and its local polarisation, or electric potential difference. This effect is caused by the dipoles present in lipid molecules. When a lipid bilayer is curved a local polarisation is induced, causing a transmembrane potential difference. The effect goes in both directions, meaning that externally applied electric potentials also induce a mechanical response in the bilayer in the form of spontaneous curvature.

Another mechanism is that of locally applying Ca^{2+} ions to one leaflet of a compositionally symmetric lipid bilayer with a negative surface charge, which induces tubular invaginations away from the ions. The overall mechanism is similar to the electric potential-induced curvature in the flexoelectric effect.

Here, coarse grained molecular dynamics simulations are used to study these effects, by quantifying their significance and describing the molecular mechanisms. We find that the flexoelectric effect of electric potential-induced curvature, in a simple lipid bilayer, is of biological relevance and should be taken into account at the cellular level. Furthermore, the molecular mechanism behind the induced membrane deformations from local asymmetric adsorption of Ca^{2+} ions is described.

Both effects are examples of couplings between membrane curvature and electrostatics. These phenomena have not received much attention in the literature and are therefore rarely accounted for, or incorporated, in models of cellular processes in the membranes. We hope to contribute to spreading the knowledge of these effects, since our results show that they can potentially have dominating roles at the molecular level.

These coupling effects can manifest themselves in the gating of mechanosensitive ion channels. Such channels respond to changes in the mechanical properties of the membrane, such as surface tension, which in turn, as we have shown, can be altered by application of a transmembrane electrical potential. We have initiated investigations of electric potential mediated gating of mechanosensitive channels.