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Membrane reorientation and phase transition induced by external electric fields

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Summary

Lipids in water form different structures (or phases) via self-assembly depending on hydration level of lipid. As the hydration level of lipid increases, the self-assembled structures are micelles, cylinder phase, lamellar phase, and inverted cylinder phase. Lamellar phase or bilayer is the most common structure in cells. Experiments reveal that external electric fields can induce cell membrane poration and fusion, and the technique is widely used to transfer external molecules, such as DNA and drugs, into cells.

By using molecular dynamics simulations, we studied the behaviors of pure phospholipid membrane bilayer in an external electric field, which was applied perpendicular to the initial water/membrane interfaces. Results show that external electric fields can induce membrane reorientation and phase transition. The hydration level of lipid determines the final structure. When the hydration level is 71 water per lipid (w/l), it is a lamellar to lamellar reorientation. When the hydration level is 24 w/l, it is a lamellar to inverted cylinder phase transition. The water/membrane interfaces in different final structures are parallel to the direction of the external electric field. The results are consistent with the understanding on the universe behaviors of the dielectric interface in external electric fields. Electroporation is the initial step independent of the hydration level. Deformation, fusion, fracture and pore-resealing of membrane are observed during membrane reorientation and phase transition. Complex cubic phases with 3-dimensional connections for both membrane and water appear as the intermediate structures.