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Tuning the self-assembled structures of lipid membrane by the application of external electric fields

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Summary

Micro/nano structures formed via self-assembly of biological macromolecules, such as DNA and RNA, have potential applications as building units in micro/nano/bio-devices. The self-assembled structures of biological macromolecules can be manipulated by applying electric field. Here we demonstrate such manipulation by using coarse-grained molecular dynamics simulations. Starting from randomly distributed CG DOPE lipids and polarizable water molecules, we studied the self-assembled structures in different hydration levels of lipid (the number of water molecules per lipid) and different strength of external electric fields. When the hydration level of lipid was 24 water per lipid (w/l) or 36 w/l, the self-assembled structures were lamellar bilayers. When the external electric field of 0.5 V/nm was applied on systems with different hydration levels of 24, 32 36 or 40 w/l, the self-assembled structures were inverted cylinders for the system with the hydration level of 24, 32 or 36 w/l and bilayer with pleats for the system with the hydration level of 40 w/l. When the hydration level was fixed at 36 w/l and different external electric field of 0.0, 0.1, 0.3, 0.5 or 0.7 V/nm was applied, bilayer structures could form only when the external electric field was 0.0 and 0.1 V/nm. Interestingly, the bilayer structure was curved and mirror symmetry when the external electric field was 0.1 V/nm. The curved membrane was stable during the following 150 ns after its formation at about 40 ns. Longer simulations were not performed because of the computational power limitation. The imperfect mirror-symmetric membrane also formed in the simulation with the external electric field of 0.3 V/nm, but quickly it changed to a inverted cylinder structure.