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Self-assembly of mixed lipids into bicelles and vesicles: molecular dynamics simulations. HARI SHARMA, ZILU WANG, ELENA DORMIDONTOVA, Department of Physics and Institute of Materials Science, University of Connecticut, Storrs, CT — Formation of complex supramolecular nanostructures, such as micelles, bicelles, vesicles (liposomes) etc. via self-assembly of simple molecules has provided a new pathway for the design and development of effective drug carriers. Solid nanoparticles or functional biopolymers, such as RNA, DNA, peptides can be encapsulated into these carriers for controlled delivery or selective targeting. We performed coarse grained molecular dynamics simulation using the MARTINI force field to study the self-assembly of a binary surfactant mixture composed of long and short phospholipids, DPPC and DHPC, in the ratio 3:1. We found that at low temperature lipids self-assemble into a bicelle (nanodisc) with the longer lipid mainly forming the interior and short lipid the rim of the bicelle. At higher temperature the nanodisc transforms into a vesicle with homogeneously distributed lipids. The structural changes of these nanodiscs and vesicles imposed by gold nanoparticle encapsulation and pegylation will be addressed.

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