Molecular modeling of carbon nanotubes, liposomes, polymers, and membranes for drug delivery application

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We have performed coarse-grained molecular dynamics simulations of the self-assembly of the mixture of single-walled carbon nanotubes (SWNTs) and different types of lipids, and the interactions between SWNTs and other molecules such as lipids, polyethylene glycols (PEGs), and lipid bilayers. The following topics will be presented: (1) effects of lipid structure and PEGylation on the self-assembly of lipids and SWNTs ; (2) interparticle dispersion, membrane curvature and penetration induced by SWNTs wrapped with lipids and PEGylated lipids ; (3) membrane penetration and curvature induced by SWNTs: the effect of diameter, length, and concentration ; (4) the effect of PEG size and grafting density on the conformational transition of PEGylated SWNTs between brush and mushroom. This work aids in the rational design of the size and grafting density of PEG chains to increase the drug-delivery efficiency for applications in nanomedicine.