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Direct simulation of amphiphilic nanoparticle mediated membrane interactions MUKARRAM TAHIR, ALFREDO ALEXANDER-KATZ, Massachusetts Inst of Tech-MIT — Membrane fusion is a critical step in the transport of biological cargo through membrane-bound compartments like vesicles. Membrane proteins that alleviate energy barriers for initial stalk formation and eventual rupture of the hemifusion intermediate during fusion generally assist this process. Gold nanoparticles functionalized with a combination of hydrophobic and hydrophilic alkanethiol ligands have recently been shown to induce membrane rearrangements that are similar to those associated with these fusion proteins. In this work, we utilize molecular dynamics simulation to systematically design nanoparticles that exhibit targeted interactions with membranes. We introduce a method for rapidly parameterizing nanoparticle topology for the MARTINI biomolecular force field to permit long timescale simulation of their interactions with lipid bilayers. We leverage this model to investigate how ligand chemistry governs the nanoparticle's insertion efficacy and the perturbations it generates in the membrane environment. We further demonstrate through unbiased simulations that these nanoparticles can direct the fusion of lipid assemblies such as micelles and vesicles in a manner that mimics the function of biological fusion peptides and SNARE proteins.

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