Abstract Submitted
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Lipid tail protrusions initiate spontaneous insertion of charged, amphiphilic nanoparticles into lipid bilayers REID VAN LEHN, MIT, MARIA RICCI, RANDY CARNEY, KISLON VOITCHOVSKY, FRANCESCO STELLACCI, EPFL, ALFREDO ALEXANDER-KATZ, MIT — Vesicle fusion is a primary mechanism used to mediate the uptake and trafficking of materials both into and between cells. The pathway of vesicle fusion involves the formation of a lipid stalk in which the hydrophobic core regions of two closely associated bilayers merge. The transition state for stalk formation requires the transient protrusion of hydrophobic lipid tails into solvent; favorable contact between these hydrophobic tails then drives stalk creation. In this work, we use unbiased atomistic molecular dynamics simulations to show that lipid tail protrusions can also induce the insertion of charged, amphiphilic nanoparticles (NPs) into lipid bilayers. As in the case of vesicle fusion, the rate-limiting step for NP-bilayer fusion is the stochastic protrusion of aliphatic lipid tails into solvent and into contact with hydrophobic material in the amphiphilic NP monolayer. We confirm our predictions with experiments on supported lipid bilayers. The strong agreement between simulation and experiments indicates that the pre-stalk transition associated with vesicle fusion may be a general mechanism for the insertion of amphiphilic nano-objects that could be prominent in biological systems given the widespread use of NPs in applications ranging from drug delivery to biosensing.

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