Supplementary Information

Internalization pathways of nanoparticles and their interaction with a vesicle

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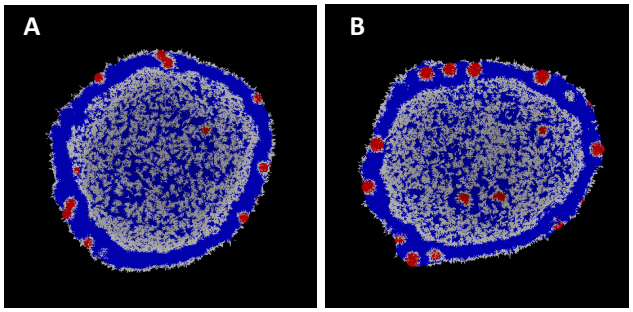

Figure S1 Pathways of NP penetration into a spherical vesicle of 37 nm with a lipid model of $H_3(T_5)_2$. (A) The pathway of cooperative chain-like penetration for 160 NPs of 2.0 nm; (B) Direct penetration for 96 NPs of 3.5 nm.

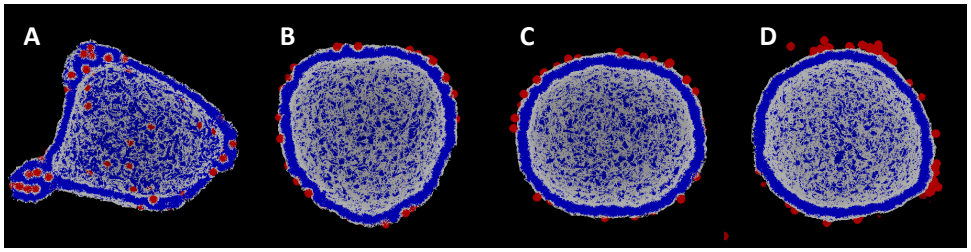

Figure S2 Effect of NP–lipid head attraction on the pathways of NP penetration. The strength of attraction between NP and lipid head decreases from a_{ph}=0 (A) , 5.0 (B), 10.0 (C) to 15.0 (D). For the snapshots, the diameter of the spherical vesicle is set to 60 nm, and 160 NPs of 3.0nm are initially adsorbed on the vesicle surface.

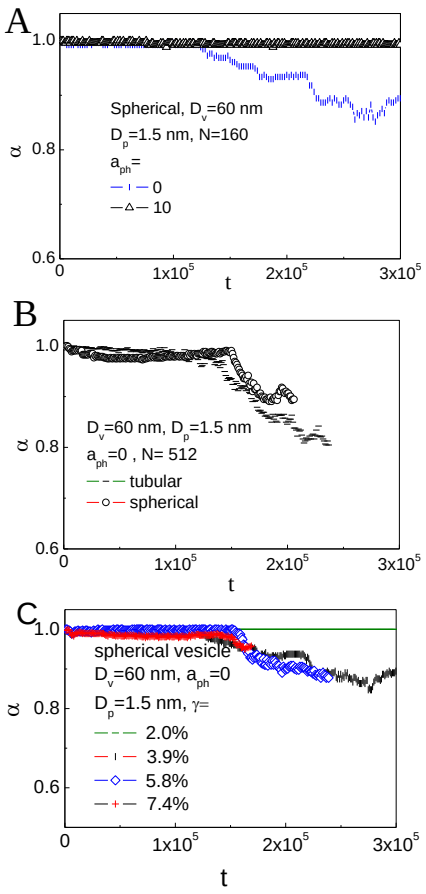

Figure S3 penetration ratio as a function of (A) NP-lipid head attraction, (B) vesicle type, and (C) NP concentration.

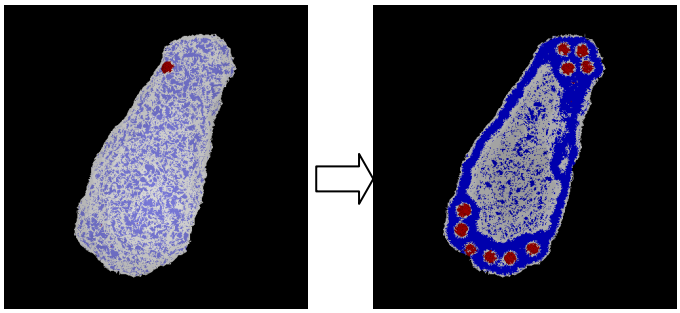

Figure S4 The formation of two protuberances for a tubular vesicle. For the system, 32 NPs of 4.5 nm are adsorbed initially on the surface of the tubular vesicle of 60 nm.