

## Quantifying Ligand Snorkeling and Membrane Partitioning of Anionic Nanoparticles: Effect of Ligand Length and Arrangement

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### Abstract

In previous studies it has been proposed that anionic ligand coated NPs may insert into and fuse with lipid bilayers<sup>1</sup>. This is facilitated by the NP adopting a stable position in the bilayer by the snorkeling of charged ligand end groups to the surface of the bilayer<sup>1</sup>. In this study, we investigate both ligand snorkeling and the propensity of NPs to approach the lipid bilayer as a function of ligand length and surface pattern in pure DPPC bilayers. These objectives are addressed by conducting 440 ns coarse-grained molecular dynamics (CG MD) simulations on different NPs. All NPs are investigated with initial configurations either inside the bilayer and in the water phase. We show that the snorkeling position of the NPs varies with ligand length. We also show that ligand configuration influences the rate at which the NP approaches the bilayer without significantly affecting the equilibrium position of the NP at the surface of the bilayer. New tools were developed in order to quantify the snorkeling effect and the position of the NP in the water phase.

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<sup>1</sup> Van Lehn, R. C.; Atukorale, P. U.; Carney, R. P.; Yang, Y.-S.; Stellacci, F.; Irvine, D. J.; Alexander-Katz, A., Effect of Particle Diameter and Surface Composition on the Spontaneous Fusion of Monolayer-Protected Gold Nanoparticles with Lipid Bilayers. *Nano Letters* **2013**, *13* (9), 4060-4067. DOI: 10.1021/nl401365n.