

Permeation of Monolayer Coated Gold Nanoparticle across Lipid Bilayer

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The unique properties of gold nanoparticles (AuNPs) have attracted special interests for biomedical applications. In the biomedical applications, the AuNPs are required to permeate across biological membranes to reach target cellular compartments. Therefore, understanding of permeation mechanism of the AuNP across the biological membranes is a great issue in nano-bio research area. In this study, a coarse-grained molecular dynamics simulation of interaction of AuNPs with model biological membranes was performed. AuNPs coated with monolayer of alkane thiol ligands were used as model nanoparticles. Lipid bilayers composed of DPPC and DPPG (neutral and negatively charged phospholipids, respectively) were applied for model biological membranes. The simulation results indicate that a positively charged AuNP have more advantages than neutral or negatively charged AuNPs in terms of membrane permeation. It was also found that the axisymmetric structure of the lipid bilayer highly induce permeation of nanoparticles without disruption of the bilayer structure.

Keywords: Nanoparticle-cell interaction. Gold nanoparticle, Lipid bilayer, Molecular dynamics simulation