



## Behavior of citrate-capped ultrasmall gold nanoparticles on a supported lipid bilayer interface at atomic resolution

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Nanomaterials, have the ability to revolutionize current biomedical and biological research in regards to the development of novel therapies, with applications ranging from drug delivery, diagnostics to controlling specific biological process. Current research is aimed at specific tasks such as enhancing cellular uptake of a material whilst keeping functionality. However the specific interactions that govern interactions between nanomaterials and biological systems, in particular cellular membranes, remains vaguely understood and under-characterized. This study provides detailed insights into the molecular mechanisms that govern the fundamental interactions between one of the most commonly used nanoparticles and model phospholipid bilayers. Using a combination of atomic force microscopy (AFM) and molecular dynamics (MD) simulations, the precise mechanisms by which citrate-capped 5 nm gold nanoparticles (AuNP) interact with supported lipid bilayers (SLBs) of pure fluid (DOPC) and pure gel-phase (DPPC) phospholipids are elucidated (Figure 1). On fluid phase DOPC membranes, the AuNP are adsorbed and get progressively internalized as the citrate capping of the AuNP is “shed” or disassociated by the surrounding lipids. The AuNPs also interact with DPPC membranes, where they partially embedded into the outer leaflet, locally disturbing the lipid organization. In both systems the AuNP cause systematic perturbations throughout the bilayer. AFM shows that the lateral diffusion of the particles is several orders of magnitudes lower that that of the lipid molecules, which creates some temporary scarring of the membrane surface. These results reveal how functionalized AuNPs interact with differing biological membranes, with mechanisms that could also have cooperative membrane effects with other molecules.

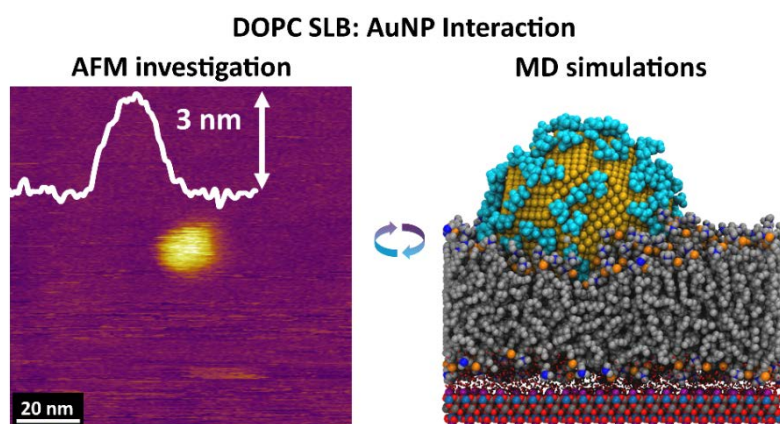


Figure 1. AFM (left) and MD simulations (right) of AuNP-SLB interaction.