# Interactions of Gold Nanoparticles and Model Membranes

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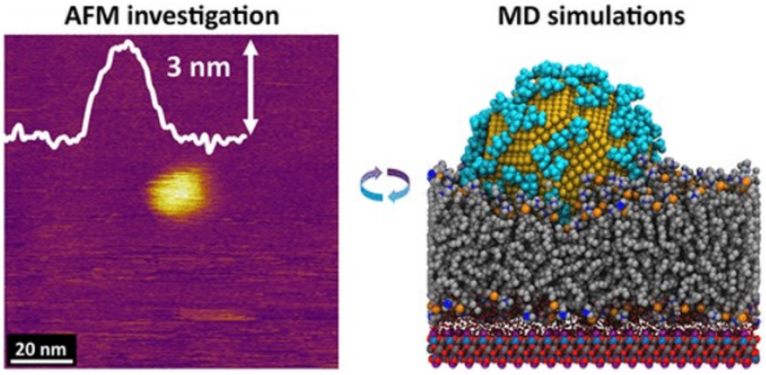
Nanoparticles (NPs) are being explored for their biomedical applications, particularly for identifying and treating disease at the cellular level. Applications of NPs include cell imaging, drug delivery and control of biological processes. To facilitate their function, NPs must interact with the cellular membrane. However, the molecular mechanisms of interaction between NPs and cellular membranes remain difficult to elucidate due to the heterogenous chemical environment of the cell membrane. For the more effective design of biomedical nanotherapeutics necessitates the need for more fundamental analysis of the interactions that govern NP and biological membranes.

This work investigates the adsorption process of various 5 nm AuNPs onto supported lipid bilayers (SLBs) using a combination of atomic force microscopy (AFM) and molecular dynamics (MD) simulations. First, the adsorption process of a citrate-coated 5 nm AuNP against homogenous fluid phase (DOPC) and gel phase (DPPC) supported lipid bilayers (SLBs) was studied. It was primarily observed that AuNP underwent easier adsorption into the fluid phase, and the dissociation of the citrate-coating facilitated the adsorption process; whilst the adsorption of the AuNPs disrupted bilayer integrity.

The adsorption capabilities of the citrate capped 5nm AuNP were then tested against a binary phase separated bilayer of fluid (DOPC) and gel (DPPC) lipids. The AuNP was observed to primarily undergo adsorption into the fluid phase domain. The AuNP adsorption also induced lateral lipid mixing and a partial dissolution of the phase boundary domain. Whilst the movement of the AuNP was primarily localized towards the phase boundary and remained in contact with both lipid phases.

Next, the role of the ligand capping agent on the adsorption process was studied. The interaction of a 5 nm AuNP capped with various strongly physiosorbed or weakly physiosorbed ligands against a fluid phase (DOPC) SLB was characterized. The weakly adsorbed ligands promoted adsorption into the SLB, whereas the more strongly adsorped ligands increase steric hinderance and shield the AuNP-surface from interacting with the bilayer inhibiting complete adsorption of the AuNP. Ligand morphology, functional group, and binding motifs of the more strongly adsorbed ligands further altered the interaction either promoting or hindering interfacial adsorption.

Finally, the role of AuNP geometry and nanoparticle concentration of the citrate capped 5nm AuNPs onto a fluid phase (DOPC) SLB was investigated. It was observed that the typical faceted nature adopted by face-centered-cubic (FCC) metallic NPs underwent adsorption quicker as compared to more spherical AuNPs, and that increasing the number of AuNPs in a SLB system increases the cost of adsorption due to increases in steric hinderance and volume exclusion effects.




*Combined atomic force microscopy and molecular dynamics simulations elucidate adsorption mechanics of gold nanoparticles onto supported lipid bilayers.*