

## **Nanoparticle-protein and nanoparticle-lipid interactions: insights from molecular dynamics simulations**

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The design of ligand-protected metal nanoparticles (NPs) with biomedical applications relies on the understanding, at the molecular level, of their interactions with different biological systems. Here we focus on gold NPs functionalized by an organic ligand shell and address their interactions with serum proteins and model cell membranes. We use molecular dynamics and enhanced sampling techniques, at atomistic and coarse-grained resolution, to characterize the molecular mechanisms and the thermodynamics of these interactions. Our results show that the interaction process is influenced by the interplay of the chemical composition of the NP ligand shell (e.g. charge and/or hydrophobicity) and by its physical conformation (e.g. folded vs extended, ordered or disordered).