# Atomistic modeling of adsorbed thiolates on Au nanoparticles (GNP). Study of the effect of the capping layer on the GNP's melting temperature.

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Metallic nanoparticles are perhaps one of the most outstanding applications of nanotechnology due to the imminent use of these nanostructures on diverse fields, i.e. biosensors, catalysis, drug "delivery" and construction of nano-circuits [1].

Preparation, conservation and protection of metallic or multimetallic nanoparticles require protection with organic ligand molecules if they will remains in a colloidal suspension. When nanoparticles are made of gold, a relatively easy way of protect them is through organic molecular self-assembly, particularly with thiolate molecules due to the strong interaction between sulfur and gold atoms. Self-assembly monolayer's (SAM's) have been intensively studied, at experimental and theoretical level, on extended gold (111) surfaces and small Au clusters. Nevertheless, a clear understanding about some fundamental structural aspects of passivated Au nanoparticles in the range of 1-30 nm still does not exist.

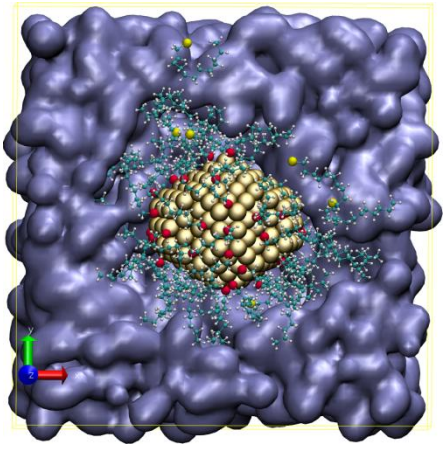

**Figura 1:** GNP (309 Au atoms) in gold-yellow. Thiolate molecules: S [Yellow (adsorbed), Red (Desorved)]. Alkyl chain in cyan (C) and white (H). Hexane solvent in continuos iceblue.

In the present work we evaluate the effect on melting temperature on GNPs where the defects induced by thiolate capping on the metallic surface are not negligible. With that in mind we have developed a many-body potential compatible with TB-SMA, to take into to account the most archetypical adsorption sites of thiolates on gold [2]. Molecular Dynamics simulations are performed to compute the thermal behavior of GNP covered with alkane thiolate on hexane. The melting point if correlated as a function of the length of thiolate alkyl chain and compared to the particle only in solvent and in vacuum [3]. The new semiempirical framework which is implemented in the TINKER code.

## References

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