

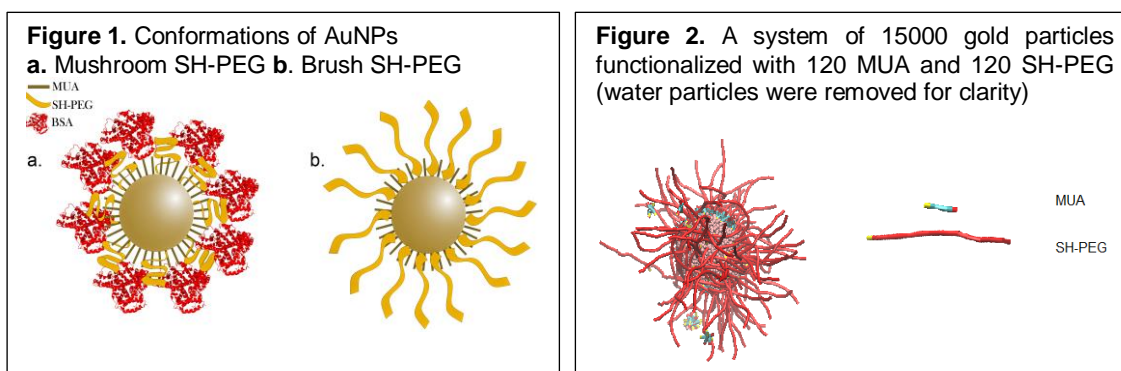
UNDERSTANDING THE BEHAVIOUR OF MULTIFUNCTIONAL GOLD NANOPARTICLES (AuNPs)

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Inorganic nanoparticles (NPs) have been used as vehicles for different therapies such as carriers for drug delivery [1], as contrast agents for imaging [2], and as radiosensitizers for radiotherapy [3]. PEG is a regular coating of nanomedicines and that conformational changes of the PEG attached to the NP have been correlated to altered biodistribution and appearance of toxicity. The aim of this study is to understand the change of the SH-PEG conformation from mushroom to brush in the mixed monolayer, which will allow further engineering of the NP surface.



The dissipative particle dynamics (DPD) [4] method was used to simulate a system containing AuNPs functionalized with 11-Mercaptoundecanoic acid (MUA) and thiolated polyethylene glycol (SH-PEG). The composition of the layer determines the physicochemical properties of the AuNPs. The competition between the MUA and SH-PEG on the surface of the nanoparticle is the key point to understand these systems.

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