Decoration of Gold Nanoparticles with Cysteine in Solution: Reactive Molecular Dynamics Simulations

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Figure 2S: Different views of the final configuration of the AuNP (887 atoms – about 0.3 nm diameter) functionalized with 164 cysteine molecules (blue/purple surfaces). a) Only the adsorbates within 0.35 nm of the AuNP (yellow surface) are shown as purple surfaces. b) All cysteines are displayed. Solvent molecules have been removed for clarity

Figure 3S: Cysteine-cysteine distances considering their alpha carbon atoms. Distances are in nm. Molecules within 0.6 nm belong to blue areas. The map suggests that all molecules are well distributed all around the AuNP.

Figure 4S: A few typical binding modes of cysteine on the AuNP
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