Electronic Supplementary Material (ESI) for Nanoscale.

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

Susanna Monti[†#*], Vincenzo Carravetta[‡], Hans Ågren[†]

[†]*Theoretical Chemistry and Biology, School of Biotechnology, KTH Royal Institute of Technology, SE-10044 Stockholm, Sweden,* [‡]*CNR-IPCF, Institute of Chemical and Physical Processes, via G. Moruzzi 1, I-56124 Pisa, Italy, and* [#]*CNR-ICCOM , Institute of Chemistry of Organometallic Compounds, via G. Moruzzi 1, I-56124 Pisa, Italy*

E-mail: sapeptides@gmail.com

Table of Contents

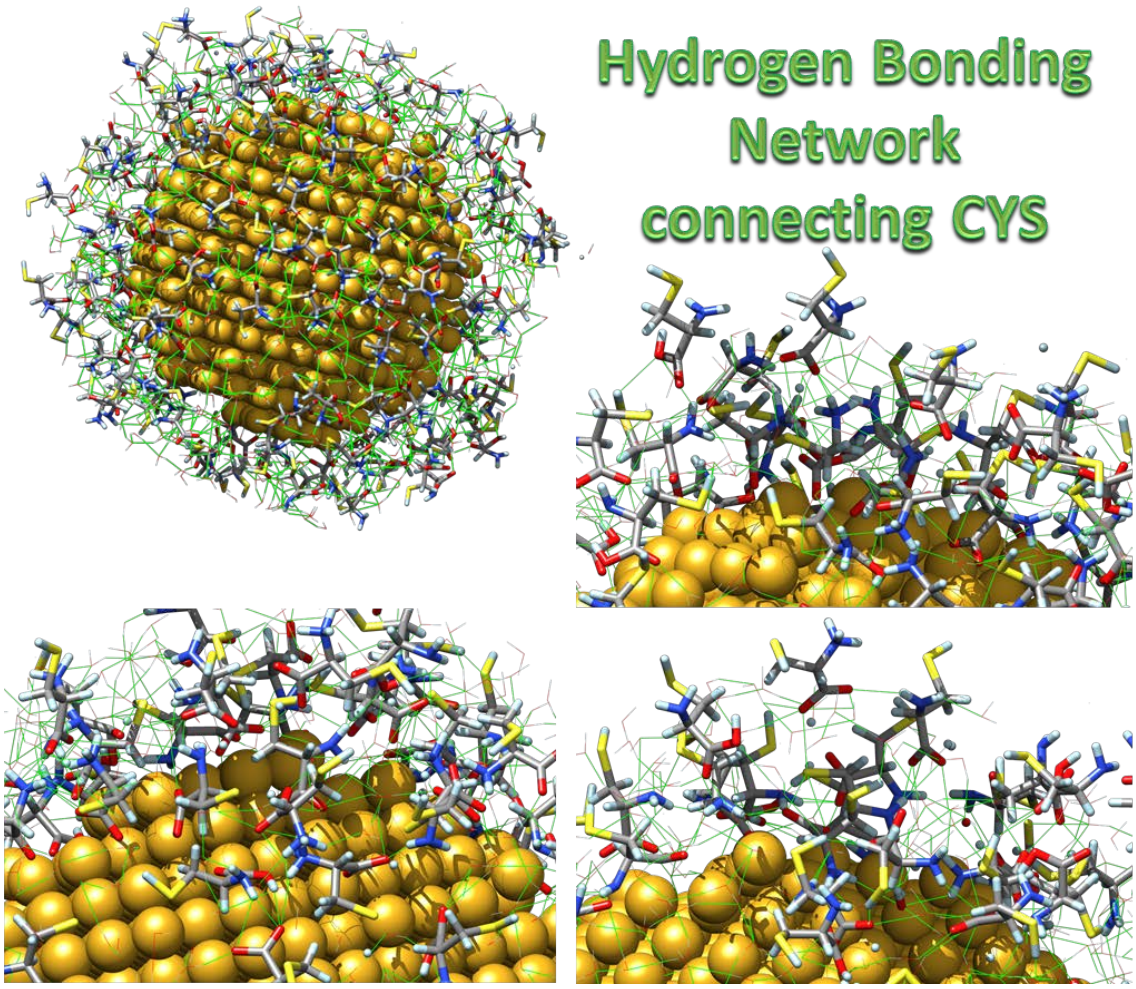

Figure1S: Final configuration of the AuNP functionalized with CYS. The first adsorbed cysteine layer and the outer molecules are displayed (all the molecules farther than 0.7 nm from the AuNP have been undisplayed for clarity). The network of hydrogen bonds is rendered through green lines connecting the donor and acceptor atoms. As it can be noticed there are a wide variety of hydrogen bonds which involve mainly the terminus groups (i.e. NH_2, NH_3^+, COOH, COO^-) but also S···HS and NH_3^+···S are observed (bottom images).

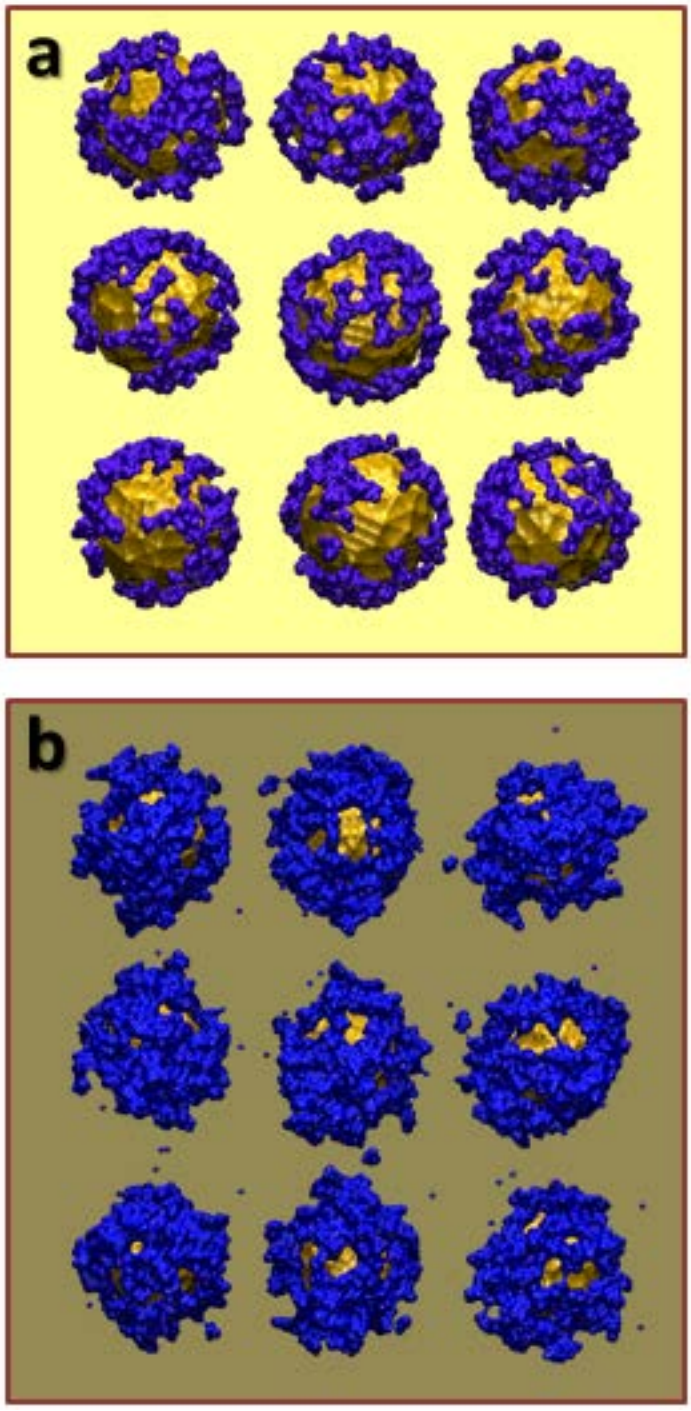

Figure 2S. Different views of the final configuration of the AuNP (887 atoms – about 0.3 nm diameter) functionalized with 164 cysteines (blue/purple surfaces). a) Only the adsorbates within 0.35 nm of the AuNP (yellow surface) are shown as purple surfaces. b) All cysteines are displayed. Solvent molecules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

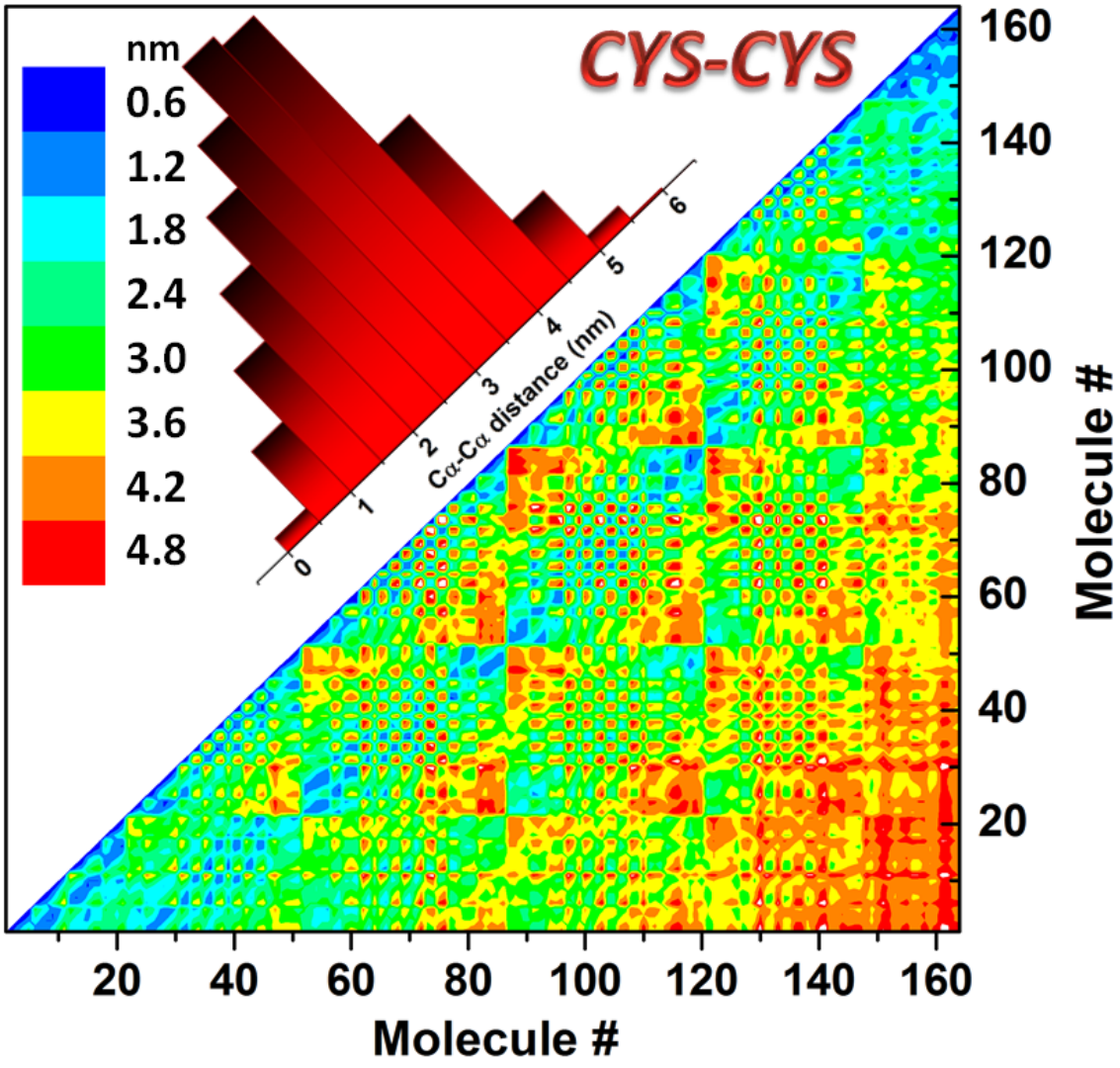

Figure 3S. Cysteine-cysteine distances considering their alpha carbon atoms. Distances are in nm. Molecules within 0.6 nm belong to blue areas. The map suggests that all molecules are well distributed all around the AuNP.

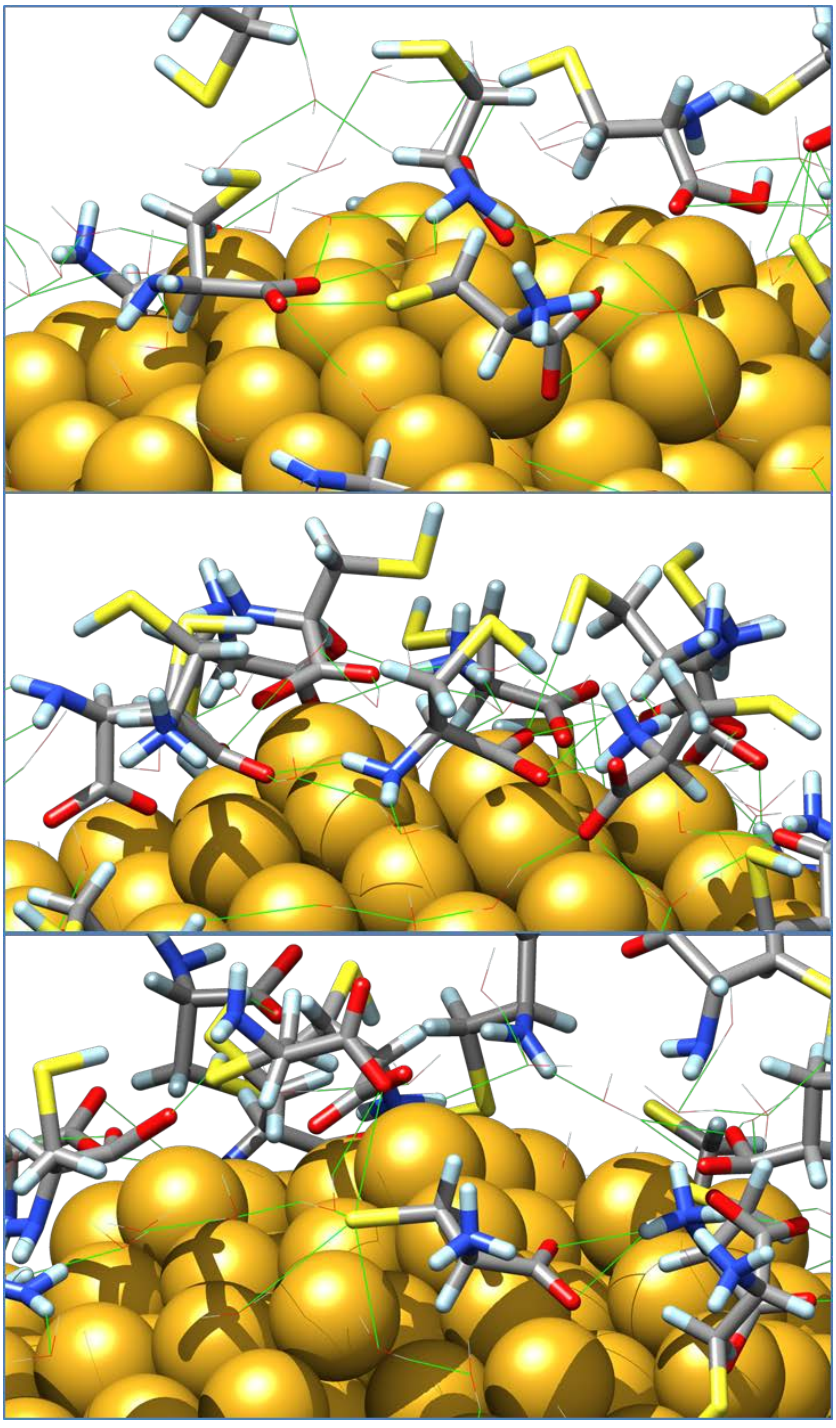

Figure 4S. A few typical binding modes of cysteine on the AuNP