Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supplementary Information to

Interaction between functionalized gold nanoparticles in physiological saline

Shada A Alsharif, Liao Y Chen, Alfredo Tlahuice-Flores, Robert L Whetten, and Miguel Jose Yacaman

In Fig. S1, we illustrate the structures of glutathione, cysteine, para-aminothiophenol, and thiophenol.

In Figs. S2 and S3, we illustrate two examples of building AuNPs: S2 for GS-AuNP and S3 for CyS-AuNP.

In Fig. S4, we show the RMSD of Au atoms in equilibrium AuNP solution from their crystallographic structure. The diffusion and rotation of the AuNP were removed when computing the RMSD, which contains only the structural deformation as compared with the crystallographic structure.

In Figs. S5 to S9, we show the work curves along the pulling paths when a pair of AuNPs are brought together in SMD simulations. Figs. S5 for a pair of two GS-AuNPs, S6 for two PhS-AuNPs, S7 for two CyS-AuNPs, S8 for pAPhS-AuNP and GS-AuNP, and S9 for two pAPhS-AuNPs.

In Fig. S10, we illustrate the distribution of Na^+ and Cl^- ions at three stages along the way of bringing the oppositely charged AuNPs together and the deformation of the Au cores when the two AuNPs are in contact with one another.

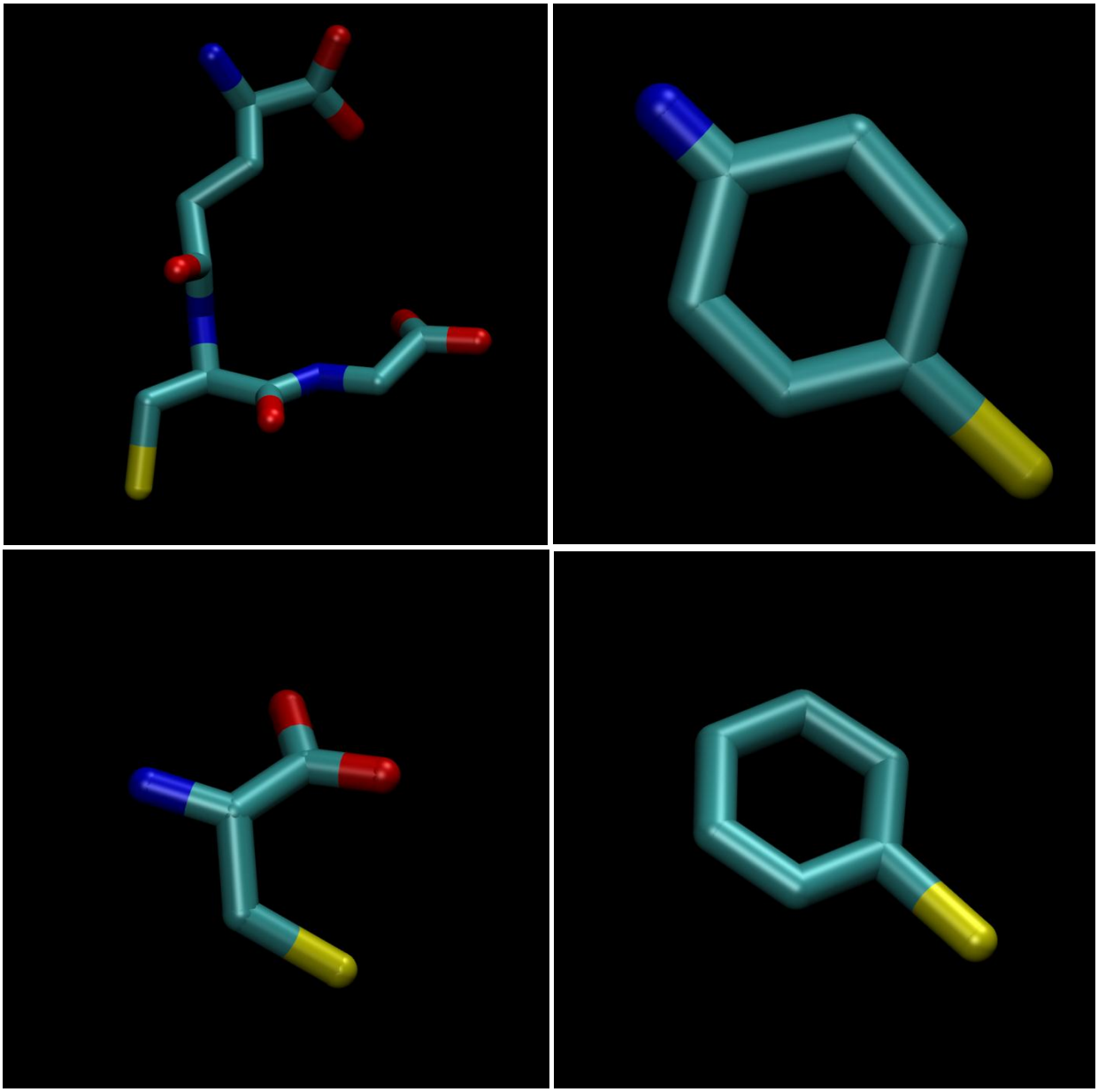

Fig. S1. Ligand structures. GS, top left. pAPhS, top right. PhS, bottom right. CyS, bottom left. S, Yellow. C, Cyan. O, Red. N, Blue.

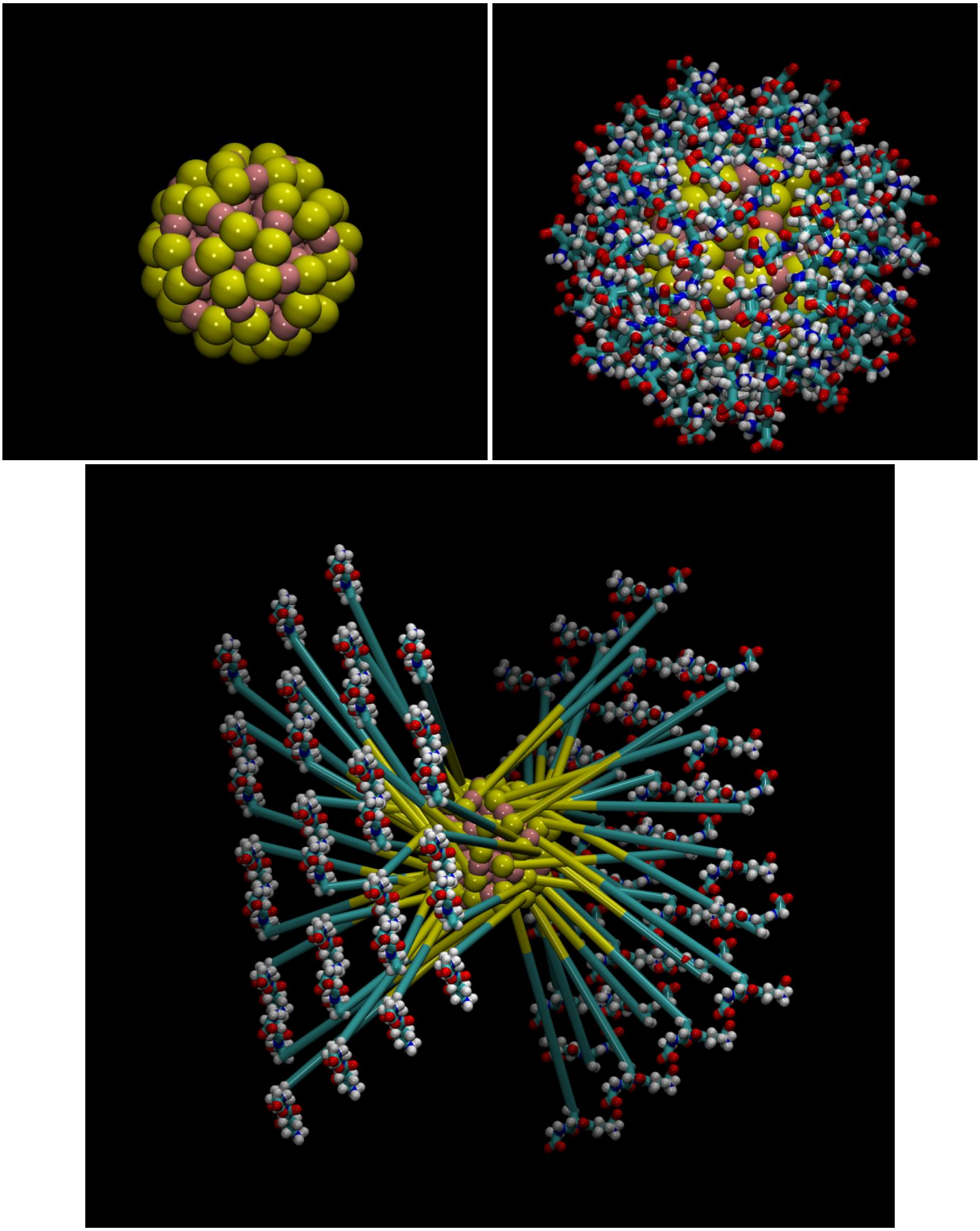

Fig. S2. (a) Shown in the top left panel is the accepted structure of the Au-S core. (b) In the bottom panel, 60 SH-less glutathiones are “bonded” to the Au-S core. (c) In the top right panel is the equilibrium structure of GS-AuNP. Both the S and Au atoms were fixed during the initial stage of equilibration.

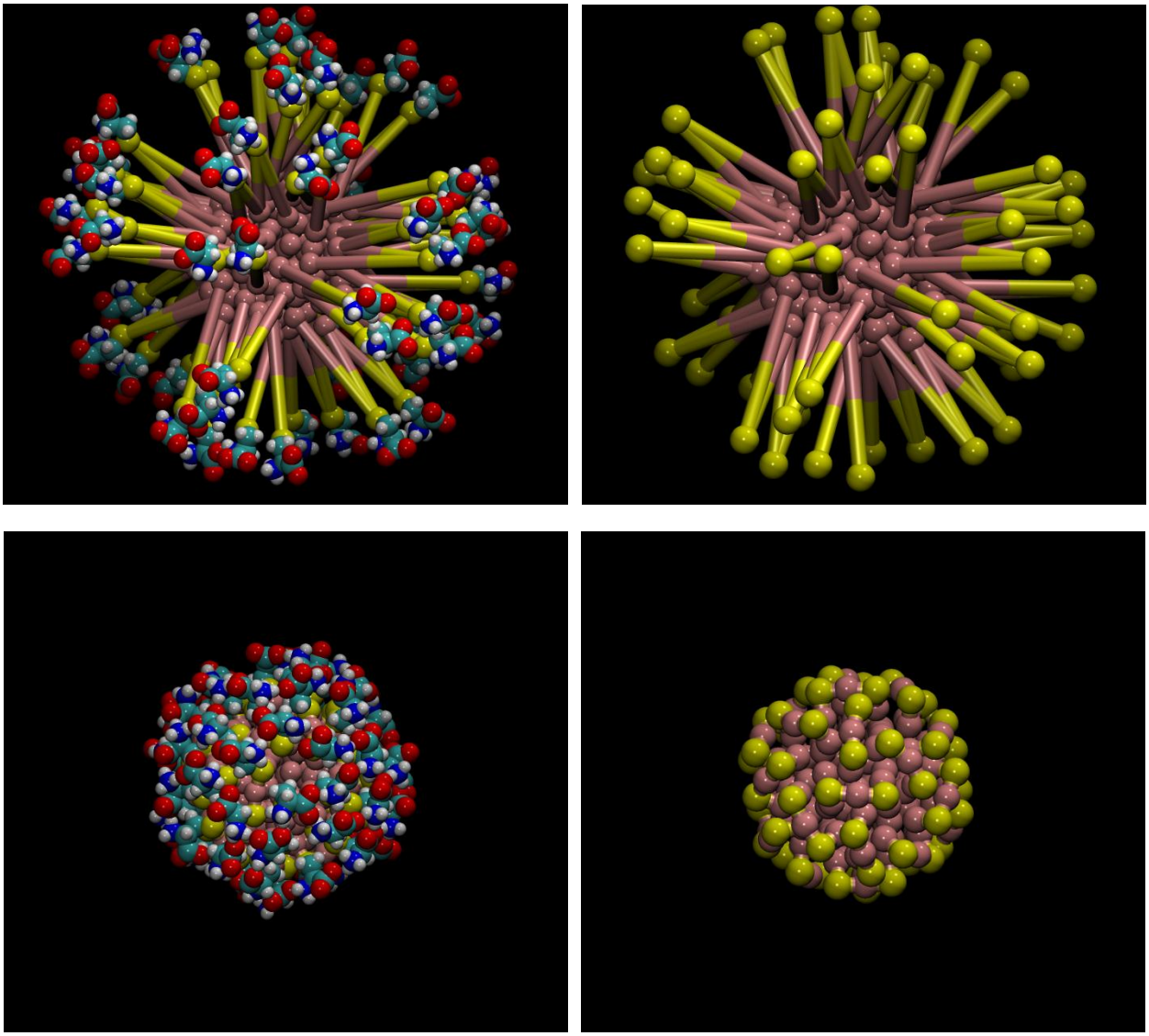

Fig. S3. (a) Shown in the top left panel are 60 H-less cysteines bonded to the Au144 core. (b) The the bottom left panel are the equilibrium structure of CyS-AuNP. (c) Top right panel (identical to (a) but only showing Au and S atoms). (d) Bottom right panel (identical to (b) but only showing Au and S atoms).

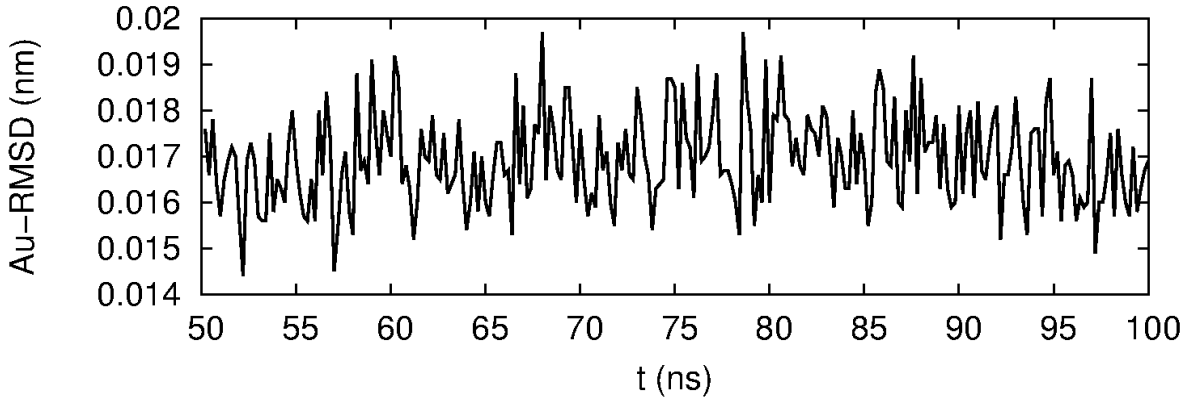

Fig. S4. RMSD of Au atoms. The reference structure coordinates are taken from Refs.58-60.

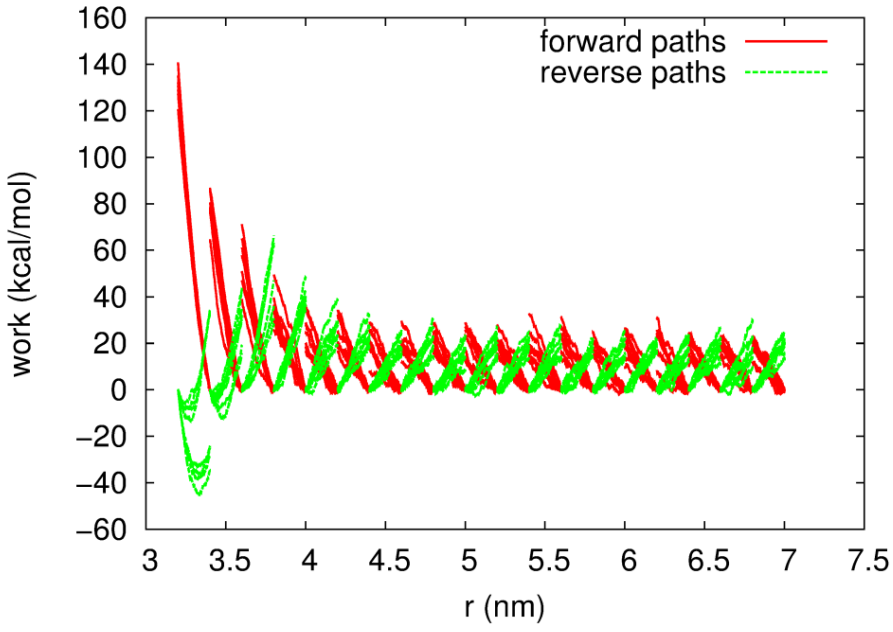

Fig. S5. Work along forward and reverse paths of pulling two GS-AuNPs together as a function of the distance r between the centers of mass of the Au cores of the two AuNPs.

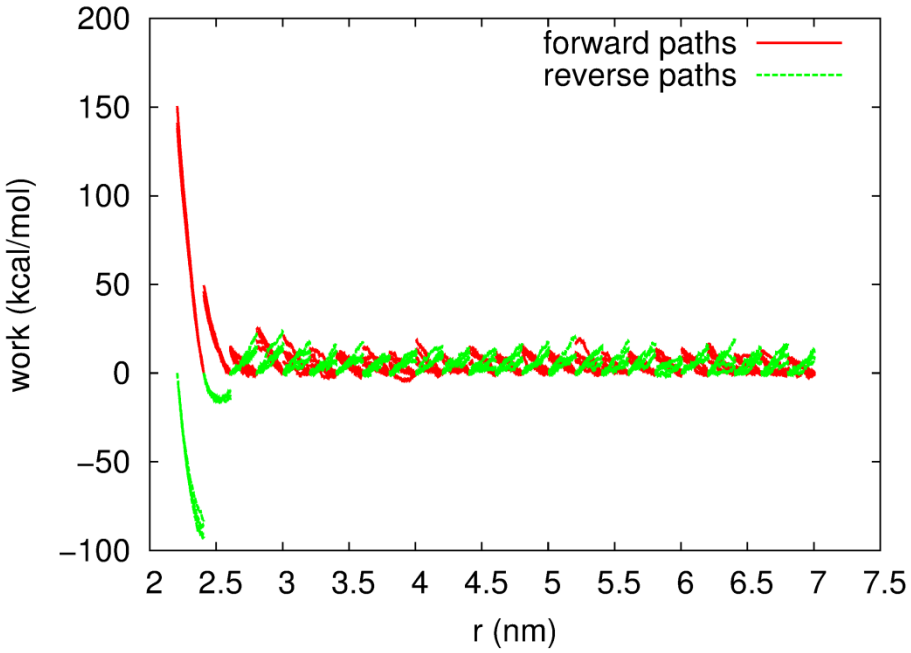

Fig. S6. Work along forward and reverse paths of pulling two PhS-AuNPs together as a function of the distance r between the centers of mass of the Au cores of the two AuNPs.

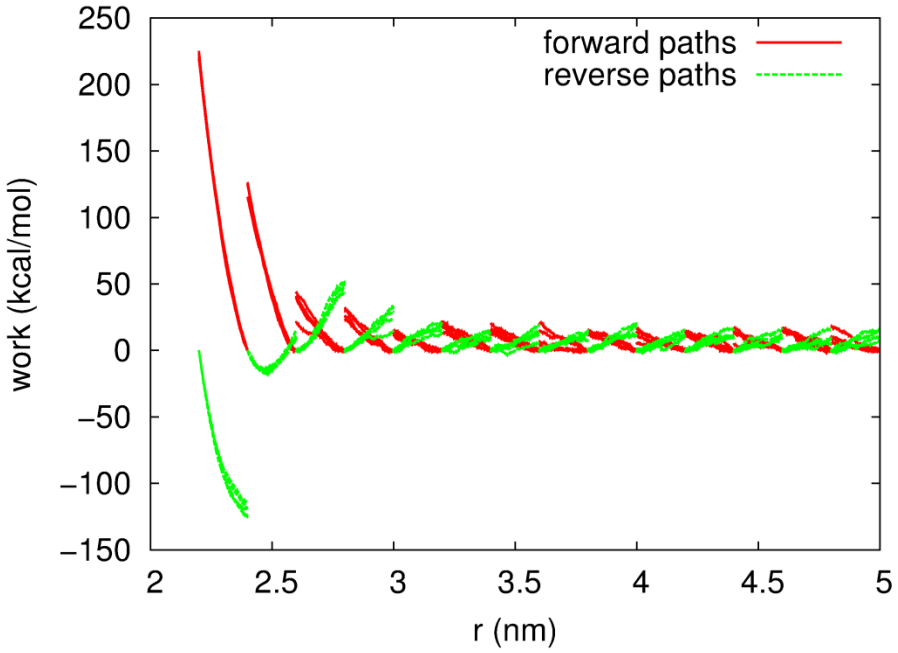

Fig. S7. Work along forward and reverse paths of pulling two CyS-AuNPs together as a function of the distance r between the centers of mass of the Au cores of the two AuNPs.

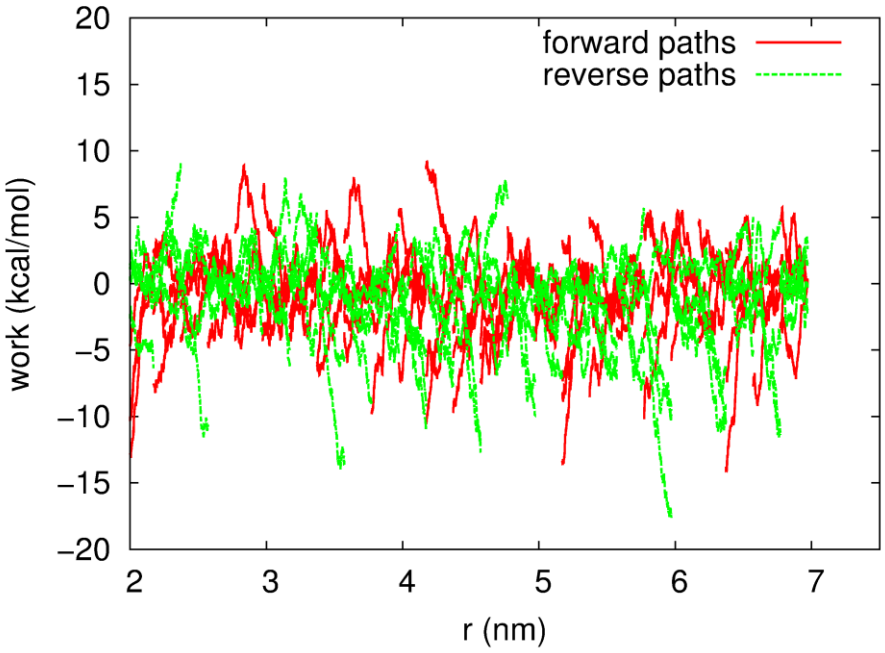

Fig. S8. Work along forward and reverse paths of pulling pAPhS-AuNP and GS-AuNP together as a function of the distance r between the centers of mass of the Au cores of the two AuNPs.

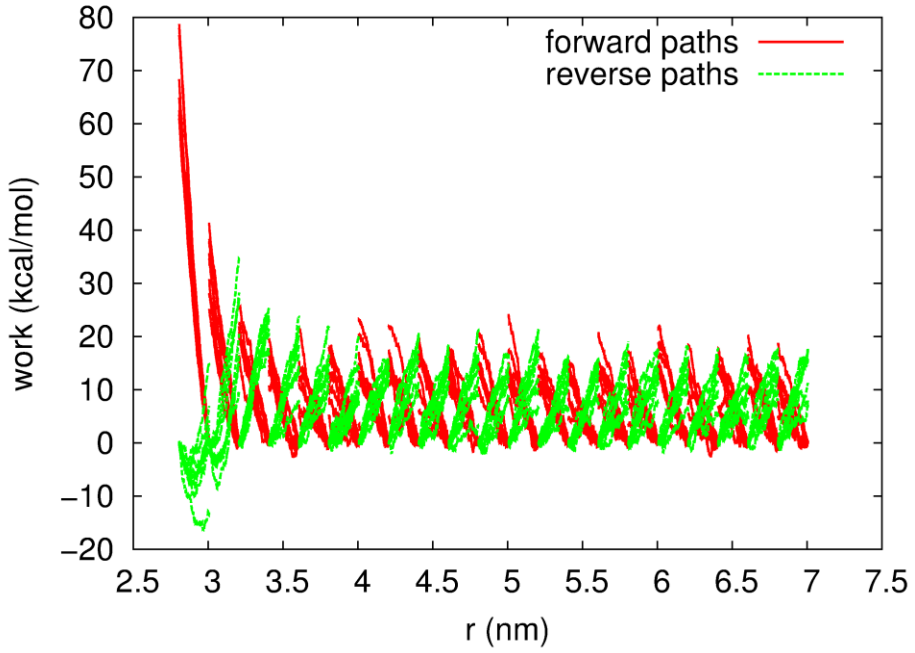

Fig. S9. Work along forward and reverse paths of pulling two pAPhS-AuNPs together as a function of the distance r between the centers of mass of the Au cores of the two AuNPs.

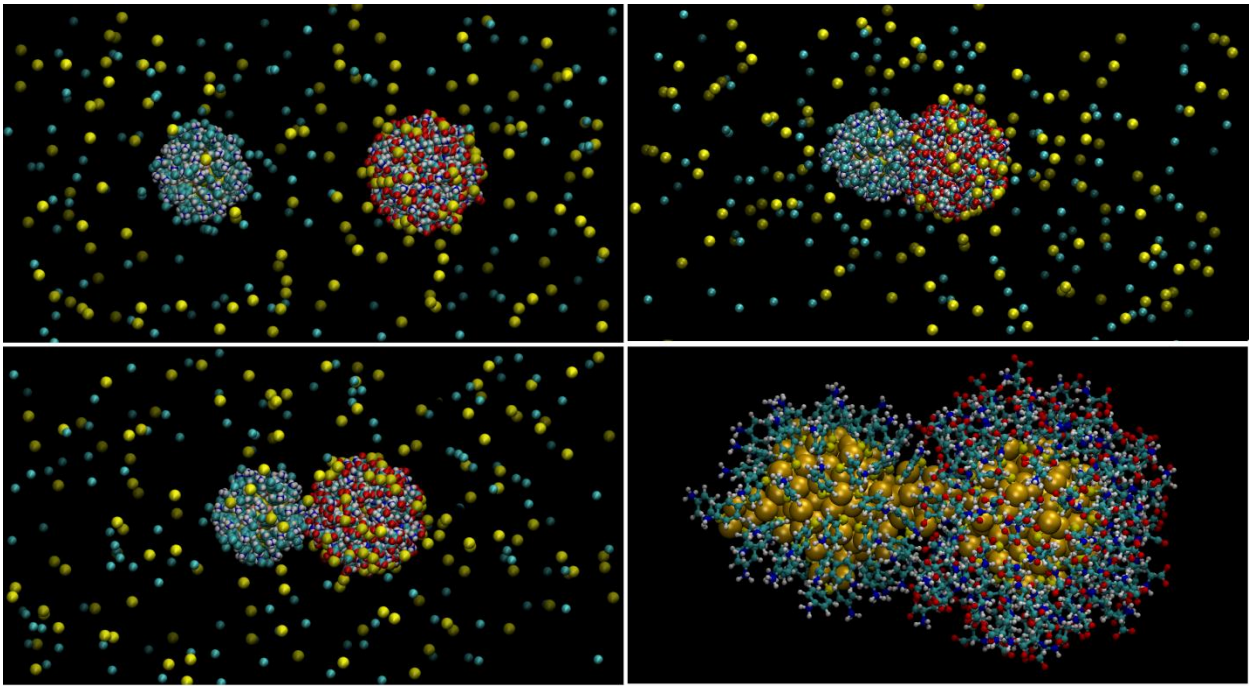

Fig. S10. pAPhS-AuNP and GS-AuNP in physiological saline when they are away from one another (top left panel, r=7 nm), in contact with one another (bottom left panel, r=3 nm), and fused together (top right panel, r=2 nm). Waters are not shown for clarity. All other atoms are in VDW representation colored by element names. In the bottom right panel is the zoom-in of the two AuNPs when they are a distance of r=2 nm where waters and ions are not shown, the Au atoms are in VDW colored in gold, and the ligand moieties (pAPhS- and GS-) are in CPK colored by element names.