Supporting Information

ReaxFF MD Simulations of Peptide-grafted Gold Nanoparticles

*Mohammadreza Samieegohar[1], Feng Sha[2], Andre Z. Clayborne[3], Tao Wei[1]**

1. Chemical Engineering Department, Howard University, 2366 Sixth Street, Washington, D.C., U.S.A, 20059

2. Network Information Center, Xiamen University of Technology, 600 Ligong Road, Jimei District, Xiamen, Fujian Province, China, 361024

3. Chemistry Department, Howard University, 525 College Street, Washington, D.C., U.S.A., 20059

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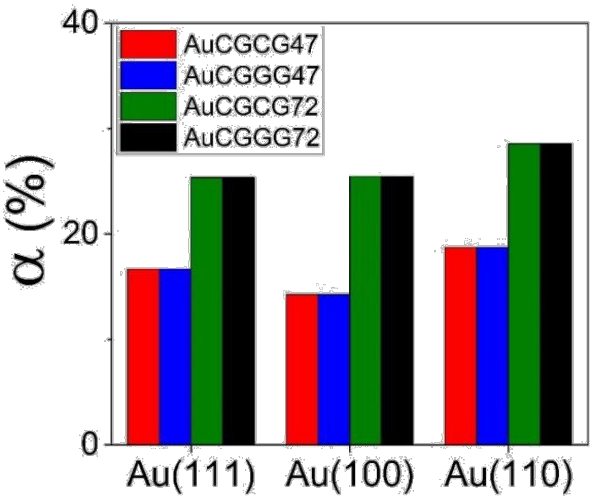

Figure S1. Initial normalized surface coverages (α) for different facets.

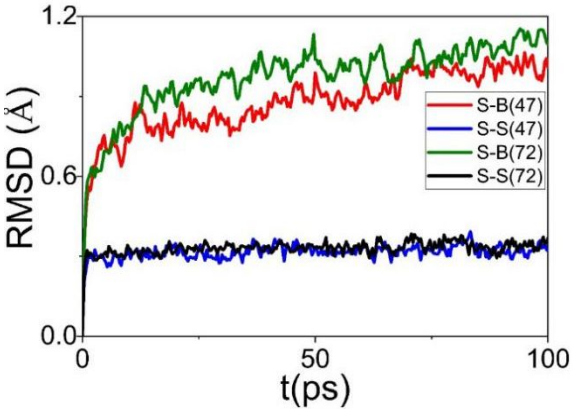

Figure S2. Root Mean Square Displacement (RMSD) for AuCGCG47 and AuCGCG72 in last 100 ps: red line: sulfur atoms away from the AuCGCG47 nanoparticle surface (S-B(47)); blue line: sulfur atoms bound on the AuCGCG47 nanoparticle surface (S-S(47)); green line: sulfur atoms away from the AuCGCG72 nanoparticle surface (S-B(72)); black line: sulfur atoms bound on the AuCGCG72 surface (S-S(72)). In RMSD calculation, the

reference configuration is the first configuration in the last 100 ps. A total of 100 configurations were sampled.

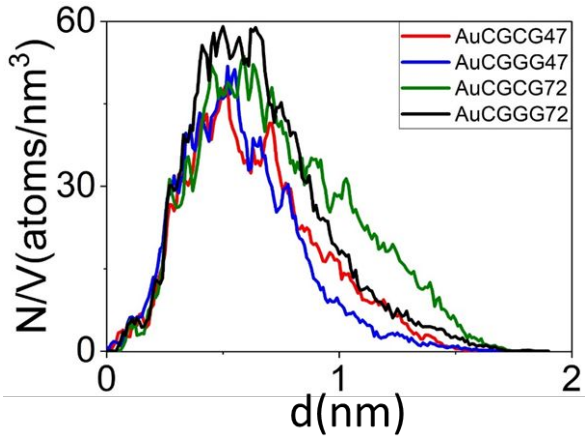

Figure S3. Peptide density profile around AuNPs by averaging 100 configurations of the last 100 ps. The distance (d) is the separation distance to the nanoparticle surfaces. Peptide SAMs thickness are: $d_{AuCGCG47}$=1.53nm, $d_{AuCGGG47}$=1.59nm, $d_{AuCGCG72}$=1.72nm, $d_{AuCGGG72}$=1.75nm.

Coarse grained simulation

Gold nanoparticle with 3 nm diameter was decorated by CGCG (Au-CGCG47) peptide in coarse grained scale and solvated in a cubic box (length 8.61 nm). Coarse grained MD simulation with Martini Force field was run for 238.3ns in NVT assemble at T=298.15K. back-mapping was used

to convert the coarse-grained structure to atomistic and the calculated gyration radius for this system was 2.21nm which is comparable with ReaxFF MD simulation.

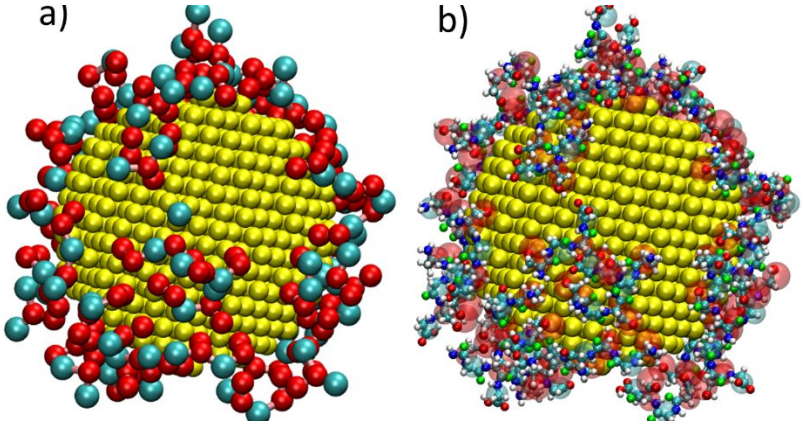

Figure S4. (a) CG simulation of AuCGCG (Au: Yellow, Cys: Cyan, Gly: Red); (b) Structure of AuCGCG47 after revers mapping to the atomistic (Au: Yellow, C: Cyan, H: White, S: Red, N: Navy, O: Green). Ghost atoms stand for Cys and Gly beads. Water molecules are removed for clear representation.