Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Monolayer Protected Gold Nanoparticles. Effect of the headgroup-Au interaction

J. A. Olmos-Asar[1,2‡], M. Ludueña[1‡] and M. M. Mariscal[1]*

[1]Departamento de Matemática y Física, Facultad de Ciencias Químicas. Universidad Nacional de Córdoba. INFIQC, CONICET. (XUA5000) Córdoba. Argentina.

[2]Dipartimento di Fisica, Università di Trieste, Strada Costiera 11, I-34151- Trieste, Italia.

Supplementary Information

Adsorption site	thiol/Au D_e	thiol/Au r_e	amine/Au D_e	amine/Au r_e
on-top (111)	0.404	2.43	0.189	2.45
on-top (100)	-	-	0.231	2.38
bridge (111)	0.271	2.64	0.058	3.23
hollow (111)	0.286	2.68	0.051	3.41
hollow (100)	0.293	2.81	0.049	3.58
top/ad-atom Au (111)	1.759	2.30	1.039	2.23
motif (RX-Au-XR)/XR	0.782	2.55	-	-

Table S1: Optimized values of the parameter D_e and r_e in the selected configurations for both, alkylthiolates and alkylamines on Au surfaces. D_e in eV units and r_e in Å.

‡ Both authors contributed equally to this work.

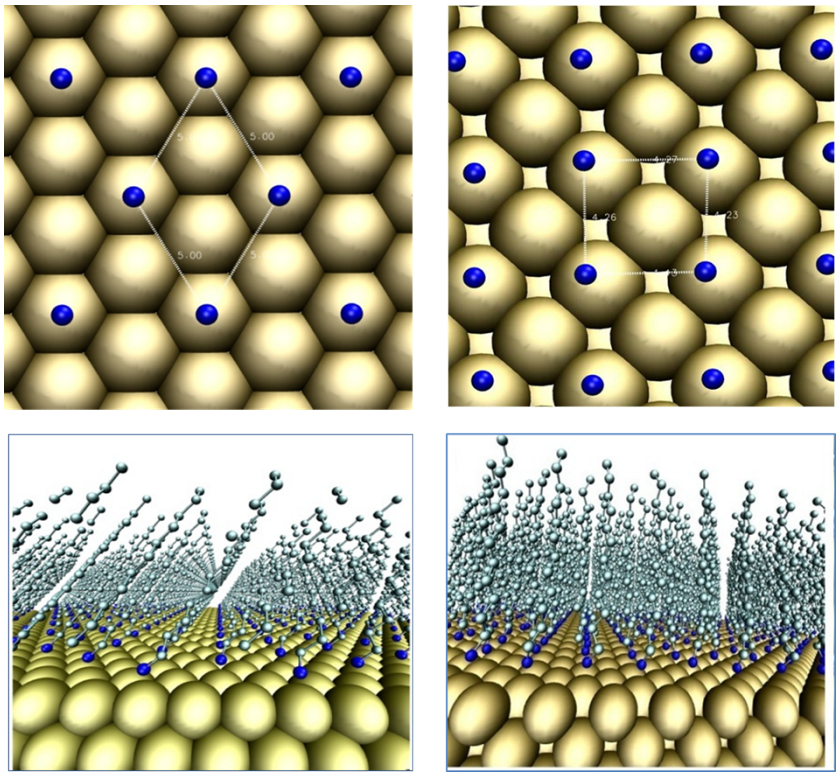

Figure S1: left) Molecular structure corresponding to a SAM of dodecanamine on Au(111) at coverage degree of θ = 0.33, which is the ($\sqrt{3}$x$\sqrt{3}$)R30º superlattice. Right) dodecanamine on Au(100) at coverage degree of θ = 0.5, which corresponds to a ($\sqrt{2}$x$\sqrt{2}$)R45º superlattice.

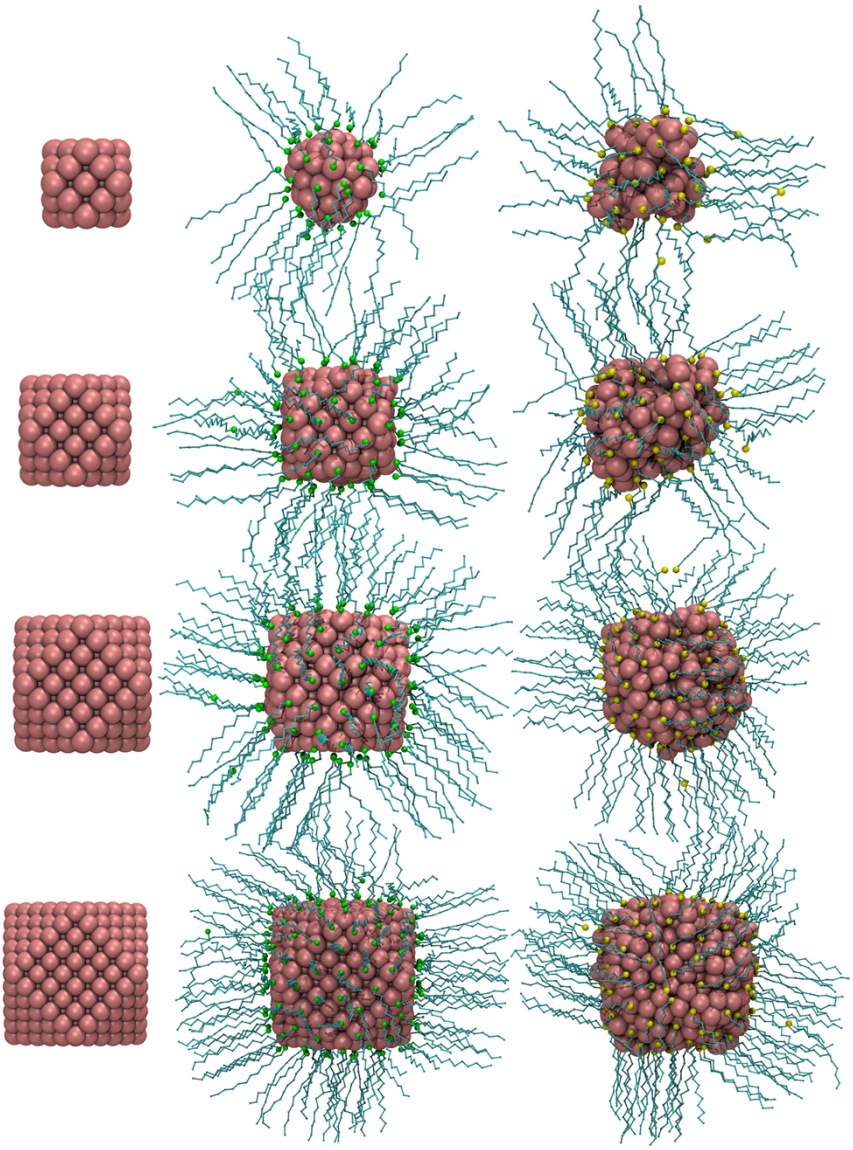

Figure S2. Atomic configuration taken from the LD simulations. Left) bare Au_N^{fcc} NPs containing N = 55, 147, 309, and 561 atoms, middle) amine-protected Au NPs, right) thiolate-protected Au NPs. (Pink spheres: Au, Green: NH_2, Yellow: S, Cian: Alkyl chains)

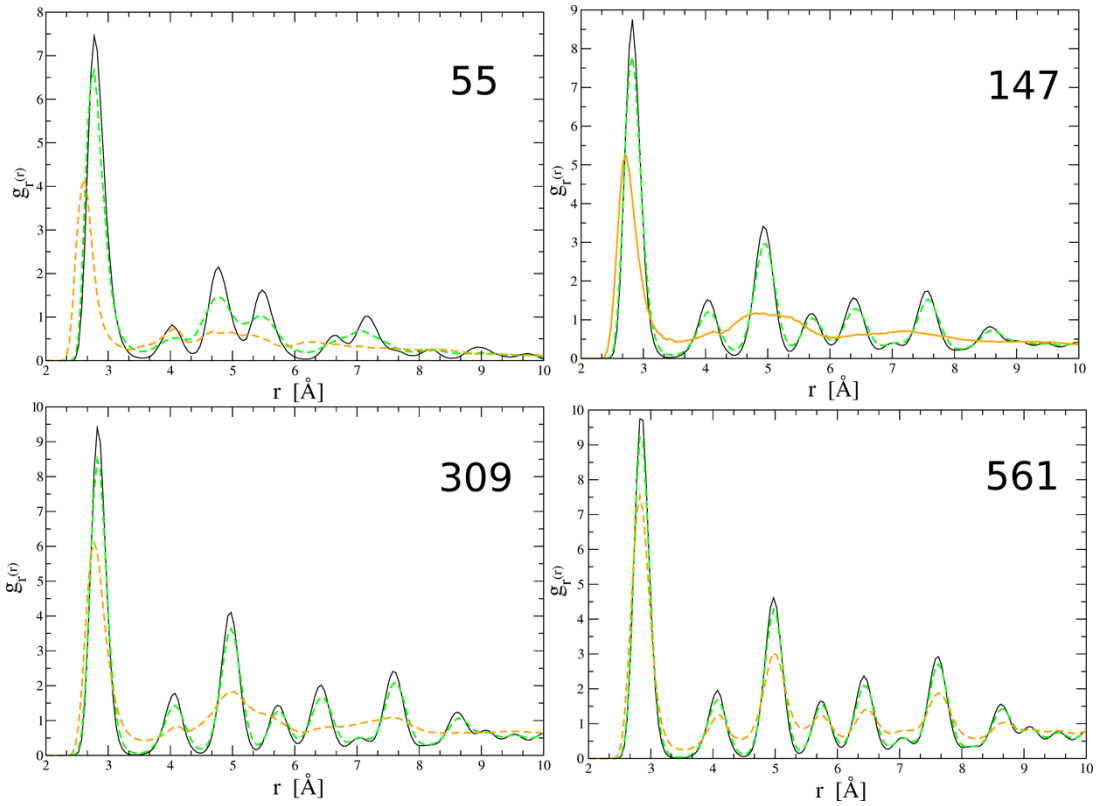

Figure S3. Pair distribution function obtained for Au-Au atom pairs. Black curves: bare Au NPs, green: amine-protected NPs, orange: thiolate-protected NPs. The numbers inside each graph correspond to the number of gold atoms in the Au_N^{fcc} NP.