Electronic Supplementary Material (ESI) for CrystEngComm.

Supporting Information

Theoretical Description of the Role of Amine Surfactant on the Anisotropic Growth of Gold Nanocrystals

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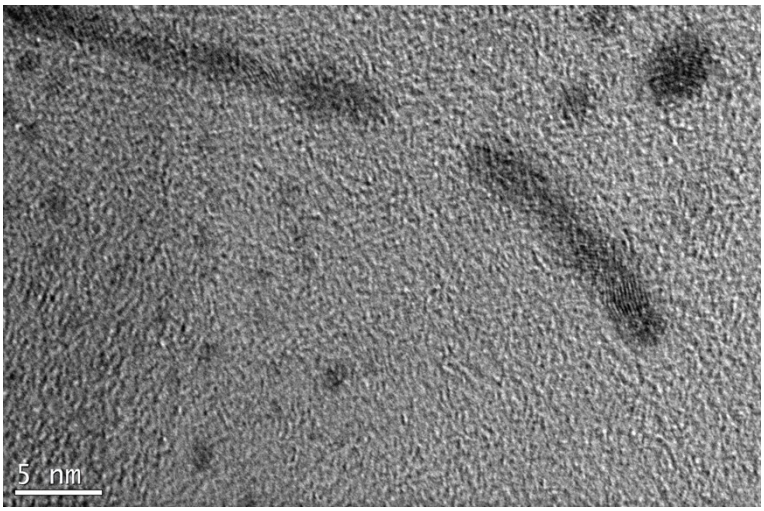

Fig. S1 TEM image of Au nanowires and nanoparticles formed in the synthetic solution after aging 24 h.

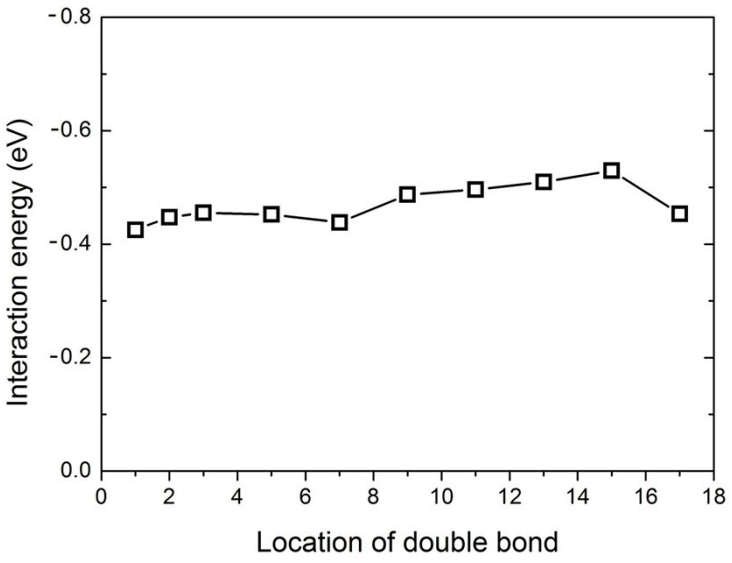

Fig. S2 Interaction energy of per molecule obtained from the aggregation of 3 amine molecules with 18 carbon-atoms-chain *vis* the position of one double band changes from 1st to 17th carbon bond neighboring to the amine functional group.

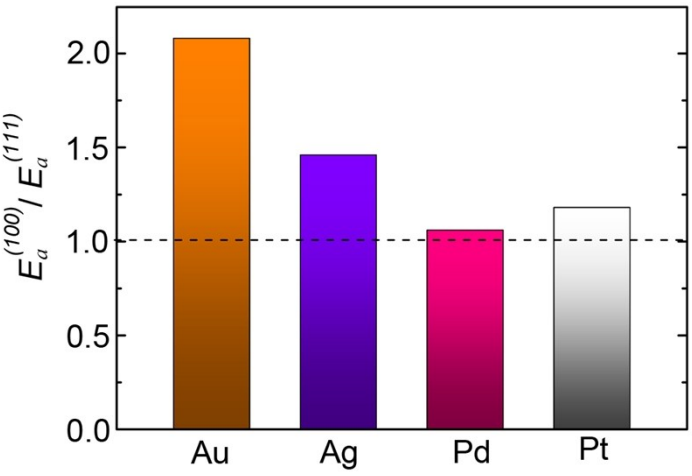

Fig. S3 Histogram for the ratio of adsorption energies ($E_a^{(100)}/E_a^{(111)}$) of amine molecule adsorbed on noble metals (Ag, Pd, Pt, Au) (100) and (111) surfaces.

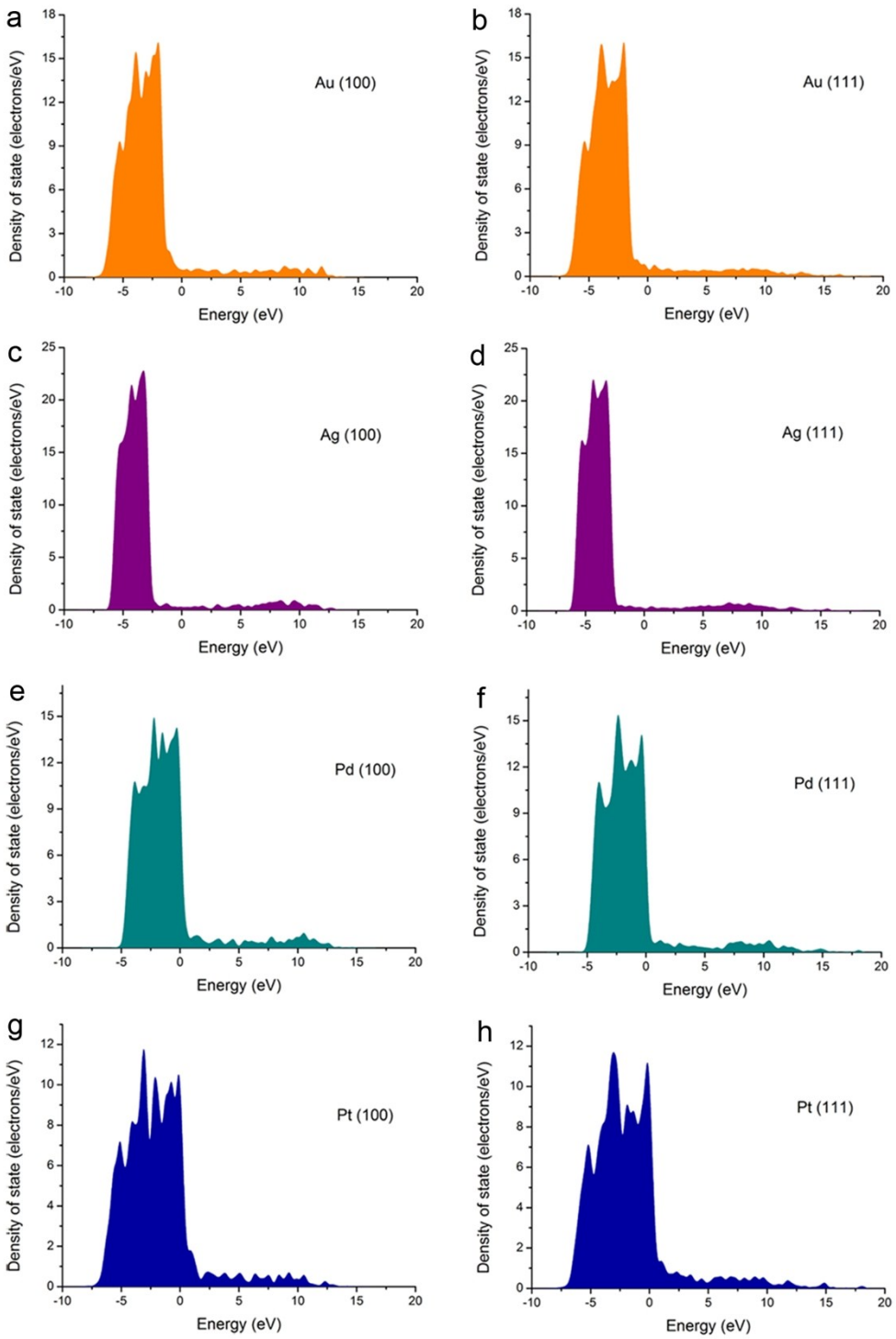

Fig. S4 Density of state (DOS) of *d*-band electrons, obtained from density functional theory (DFT) calculations, for the (a) Au (100), (b) Au (111), (c) Ag (100), (d) Ag (111), (e) Pd (100), (f) Pd (111), (g) Pt (100), and (h) Pt (111) surfaces.

Table S1. Values of *d*-Band Center Position Obtained from DOS Analysis in Fig. S4 for Noble Metals (Ag, Pd, Pt, Au) (100) and (111) Surfaces (Unit: eV).

Noble metal	(100) surface	(111) surface	Difference
Au	-3.24	-3.35	0.11
Ag	-3.95	-3.98	0.03
Pd	-1.84	-1.88	0.04
Pt	-2.21	-2.19	0.03

Table S2. Adsorption Energy of Ammonia and Methylamine molecules, Obtained from DFT Calculations, on Au (100), (111) and (110) Surfaces (Unit: eV).

Molecule	$E_a^{(100)}$	$E_a^{(111)}$	$E_a^{(110)}$
Ammonia	-0.541	-0.251	-0.551
Methylamine	-0.623	-0.298	-0.628

Table S3. Surface Energies (E_s) Obtained from DFT Calculation for Noble Metals (Ag, Pd, Pt, Au) (100), (111) and (110) Surfaces (Unit: J/m^2)

Noble metal	(100) surface	(111) surface	(110) surface
Au	1.02	0.91	1.09
Ag	1.04	1.01	1.11
Pd	1.67	1.53	1.89
Pt	2.35	2.12	2.42

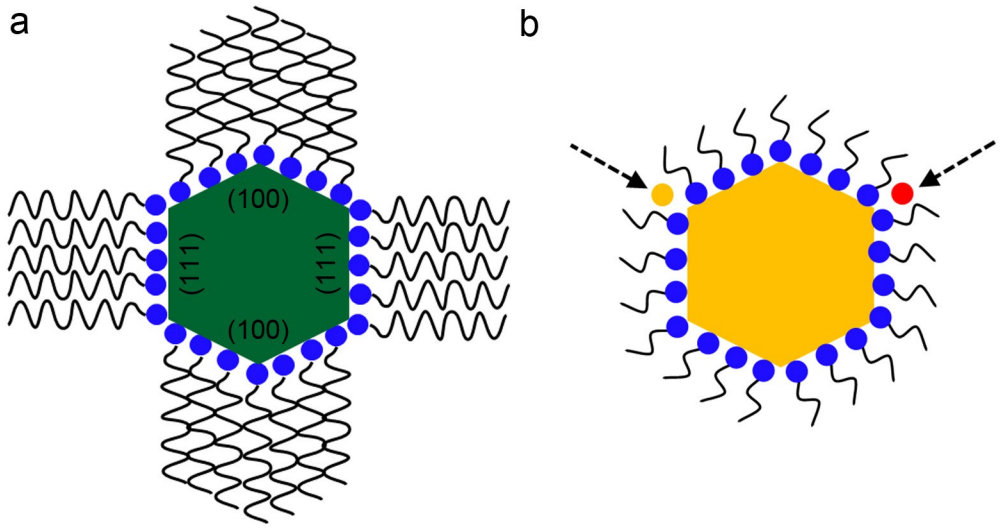

Fig. S5 Schematic image of (a) configuration of OAm molecules adsorbed on Pt or Pd nanoparticle as surfactant, and (b) Au nanoparticle adsorbed by short-carbon-chain amine molecules.