Supporting information

Solvent induced stable pseudopolymorphs of Au(I)-thiolate lamellar assemblies: a model system for understanding the environment acclimation of bio-macromolecules

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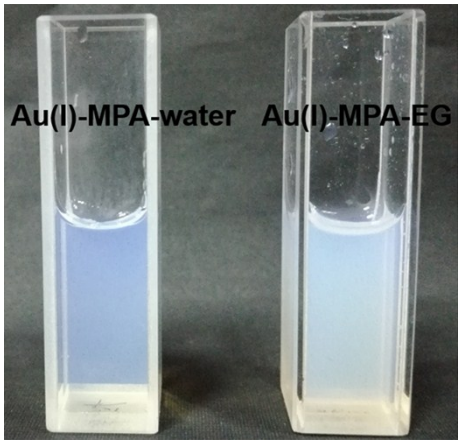

Figure S1. Optical images of Au(I)-MPA-water and Au(I)-MPA-EG assemblies in quartz cuvettes at reaction concentration ([Au]=1×10^{-3} mol·L^{-1}).

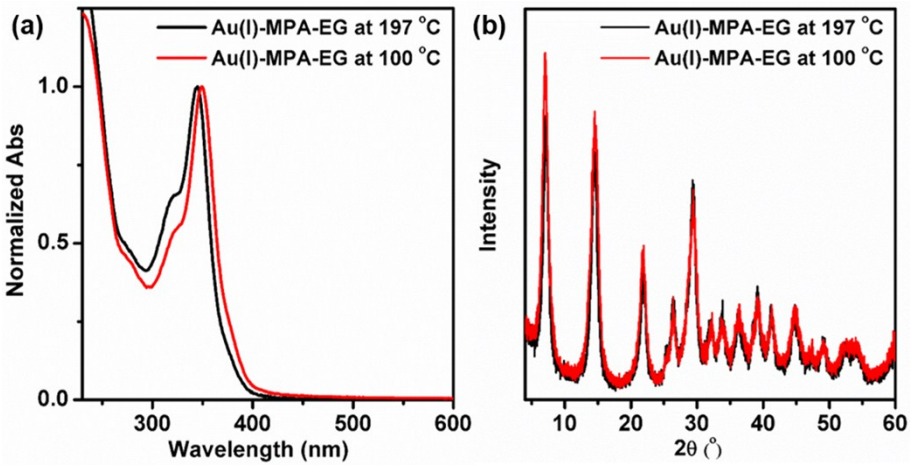

Figure S2. (a) UV-vis spectra and (b) PXRD patterns of Au(I)-MPA-EG assembled at 197 °C and 100 °C.

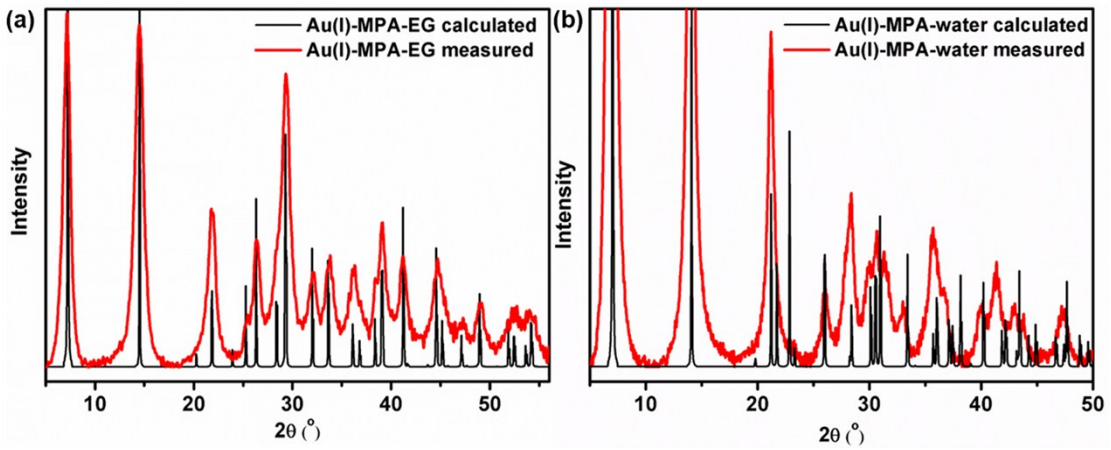

Figure S3. The calculated and measured PXRD patterns of (a) Au(I)-MPA-EG and (b) Au(I)-MPA-water assemblies. The calculated and measured PXRD for Au(I)-MPA-EG matched very well. We screened all the possible unit cell structures suggested by Jade 5 software, there is no one can perfectly match with the measured data for Au(I)-MPA-water because of their small size and thin thickness. In the best-matched one as shown in the Figure S3b, the patterns between the two are similar, but the positions deviate a little in large angle region, this suggests there may be some deviations of the crystal structure.

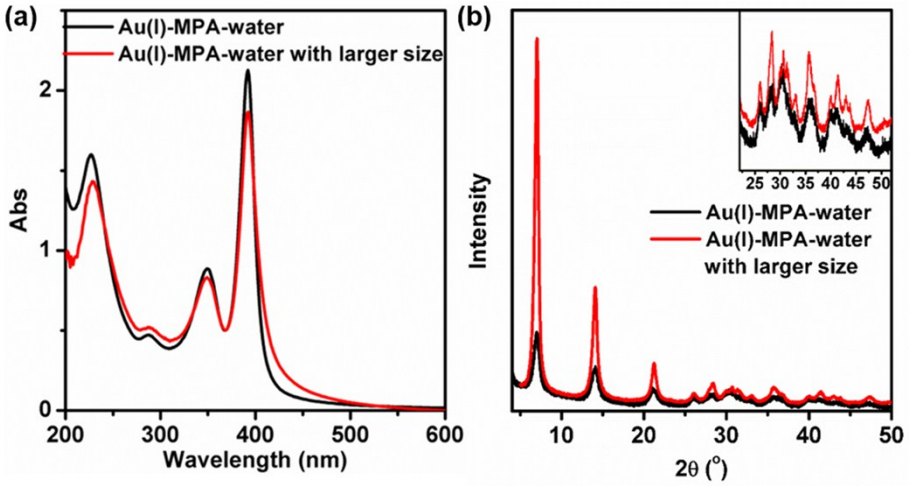

Figure S4. (a) UV-vis spectra and (b) PXRD patterns of Au(I)-MPA-water and Au(I)-MPA-water with larger sizes with special synthetic procedures.

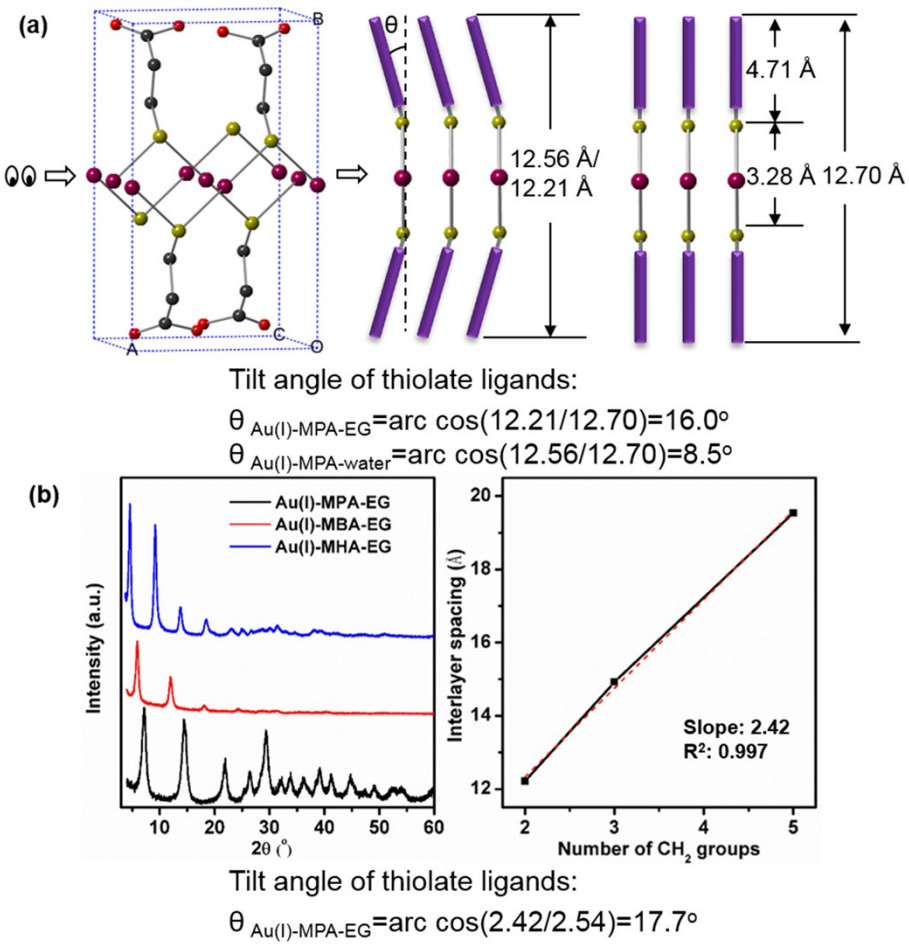

Figure S5. (a) Calculations of the tilt angle of the thiolate ligands, (b) PXRD patterns of Au(I)-nSR-EG assemblies (n=3 Au(I)-MPA-EG, n=4 Au(I)-MBA-EG and n=6 Au(I)-MHA-EG) and the measured inter-layer spacing of the assemblies as a function of the number of methylene groups. According to the literature[1], the slope of the thiolate ligands taking upright conformation is 2.54. MPA: 3-mercaptopropionic acid, MBA: 4-mercaptobutyric acid, MHA: 6-mercaptohexanoic acid.

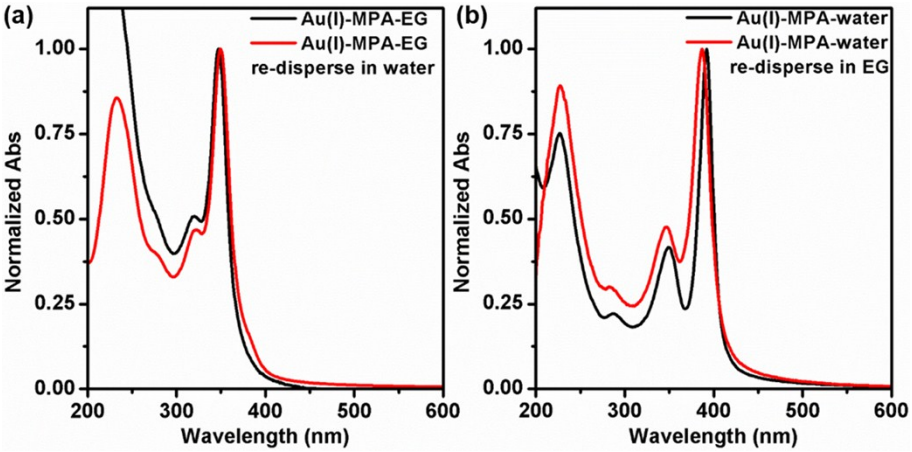

Figure S6. UV-vis spectra of (a) Au(I)-MPA-EG assemblies re-dispersed in water and (b) Au(I)-MPA-water assemblies re-dispersed in EG at room temperature.

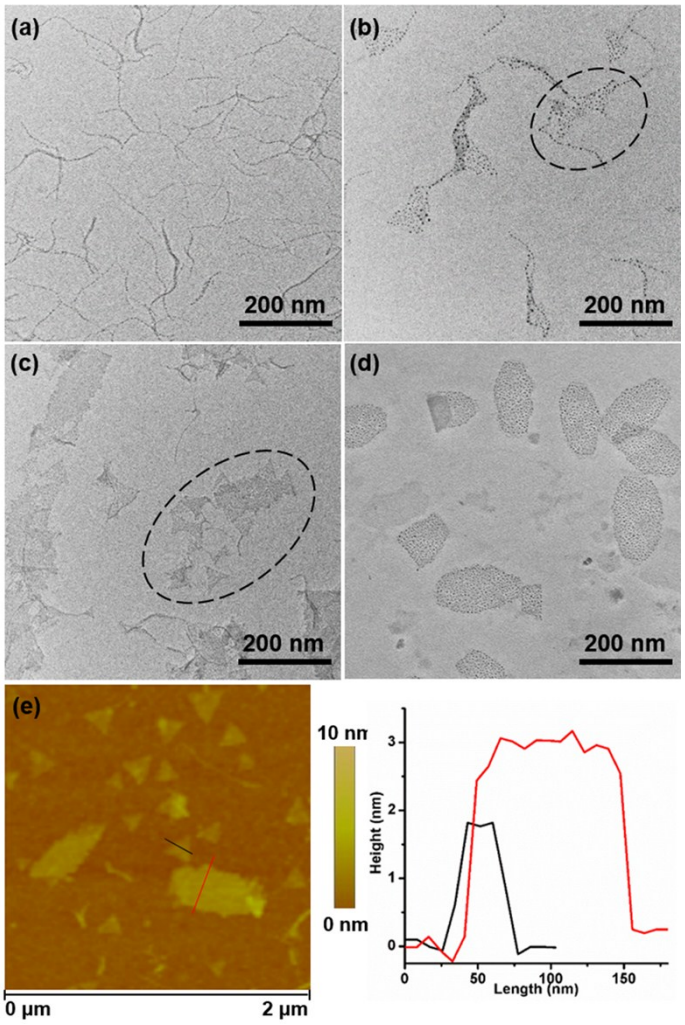

Figure S7. TEM images of Au(I)-MPA-water assembled at (a) 5 s, (b) 1 min, (c)

3 min and (d) 5 min, (e) AFM image and height analyses of Au(I)-MPA-water assembled at 3 min. The strings can aggregate and crystallize into triangular nanosheets, and the triangular nanosheets are not stable, which will further aggregate with other triangle nanosheets/strings to form larger lamellar nanosheets. It is an aggregation-growth process.

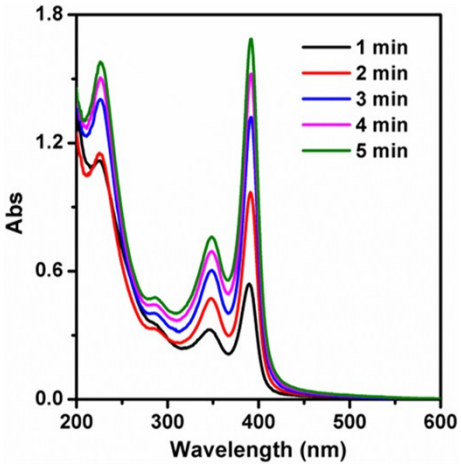

Figure S8. UV-vis spectral monitoring of the assembly process of Au(I)-MPA-water assemblies.

Table S1. XPS analyses of Au(I)-MPA-water and Au(I)-MPA-EG assemblies.

	Au(I)-MPA-water assemblies	Au(I)-MPA-EG assemblies
Binding Energy of Au $4f_{7/2}$	84.36 eV	84.34 eV
FWHM of Au 4f7/2	0.99 eV	0.97 eV
Au/S molar ratio	1.03	1.03

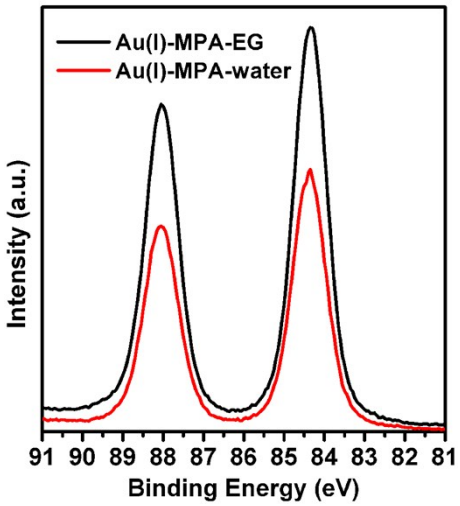

Figure S9. The high-resolution XPS spectra of the O 1s peak of Au(I)-MPA-EG and Au(I)-MPA-water assemblies.

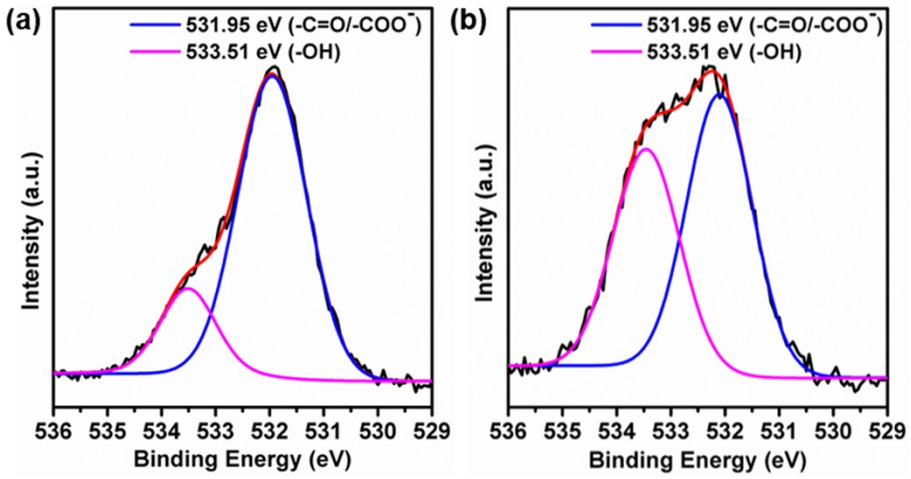

Figure S10. The high-resolution XPS spectra of the O 1s peak of (a) Au(I)-MPA-EG and (b) Au(I)-MPA-water assemblies.

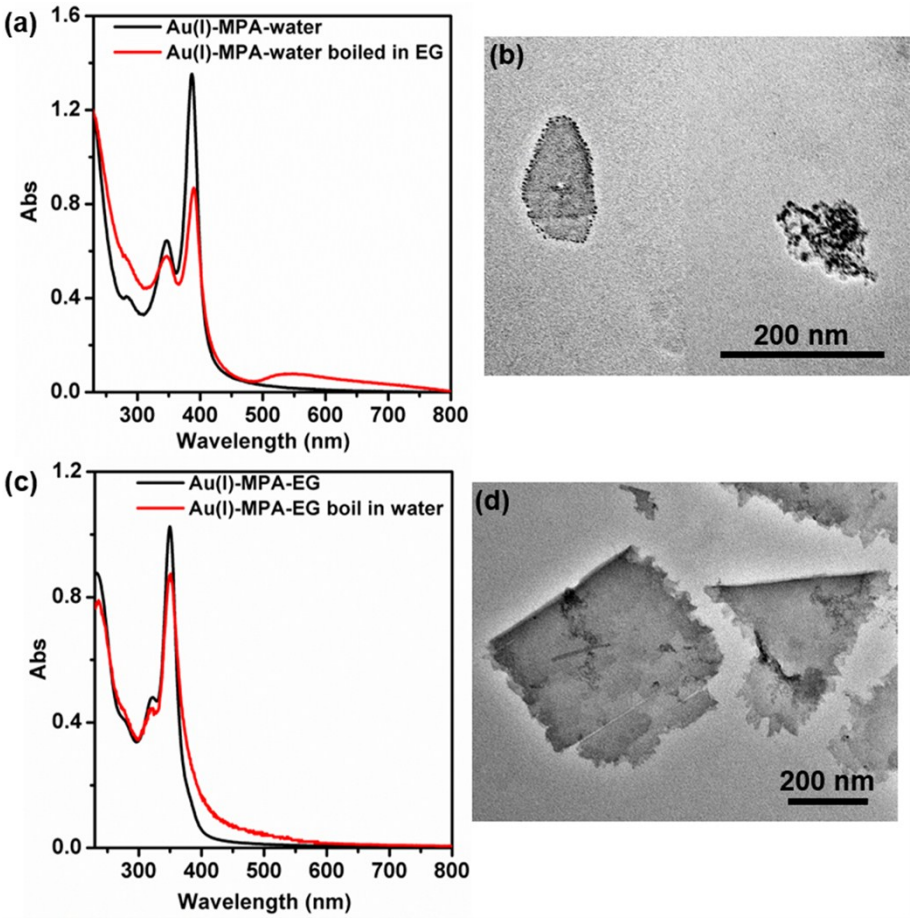

Figure S11. UV-vis spectra of Au(I)-MPA-water assemblies re-dispersed in EG and boiled for 5 min and (b) their TEM image; (c) UV-vis spectra of Au(I)-MPA-EG assemblies re-dispersed in water and boiled for 5 min and (d) their TEM images. From the TEM images, part of the Au(I)-MPA-water assemblies have been reduced into Au nanoparticles (on the edge of the nanosheets and some aggregated on the substrate) when boiled in EG. No Au nanoparticles were observed when Au(I)-MPA-EG assemblies were boiled in water, while the stronger absorption tail towards long wavelength region after further heating is mainly due to the strong light scattering, if there are any gold generated, their amount will be few.

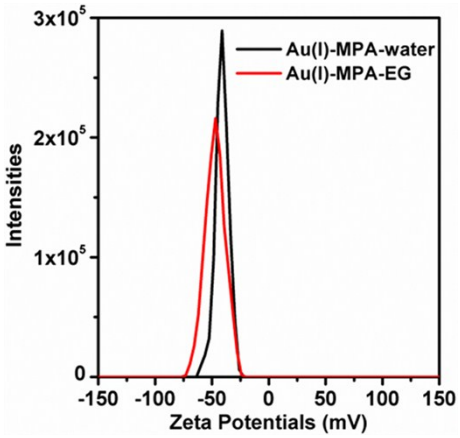

Figure S12. Zeta potentials of Au(I)-MPA-water and Au(I)-MPA-EG assemblies.

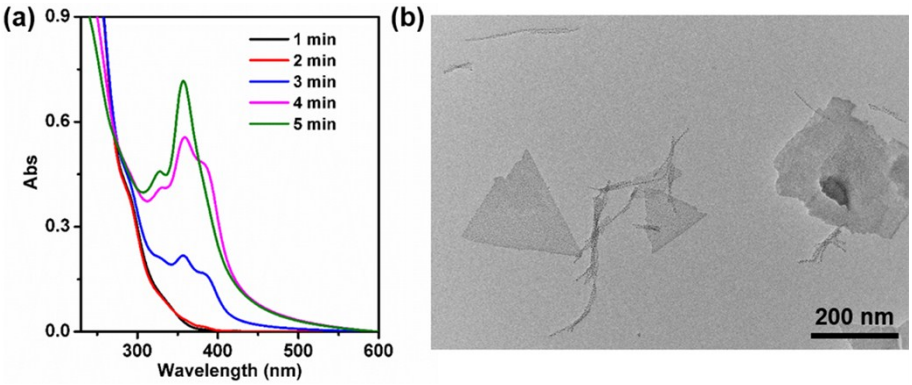

Figure S13. (a) UV-vis spectral monitoring of the assembly process of Au(I)-MPA-EG, the time was recorded when the solution began to boil; (b) TEM image of the unassembled intermediates existing in the final Au(I)-MPA-EG assemblies.

[1] S.-H. Cha, J.-U. Kim, K.-H. Kim, J.-C. Lee, *Chem. Mater.*, **2007**, *19*, 6297-6303.