Electronic Supplementary Information of

"Solution-Dispersible Au Nanocube Dimers with Largely Enhanced Two-Photon Luminescence and SERS"

Xiao-Li Liu, Shan Liang, Fan Nan, Zhong-Jian Yang, Xue-Feng Yu*, Li Zhou*, Zhong-Hua Hao and Qu-Quan Wang*

Department of Physics, School of Physics and Technology, Wuhan University, Wuhan, 430072, P.R.China.
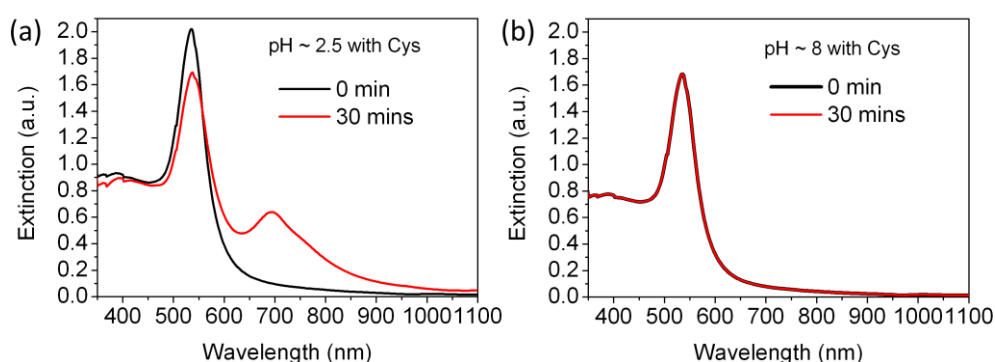

Fig. S1 Extinction spectra of the original Au nanocubes and the products with the assembly reaction time of 30 mins at pH of 2.5 (a) and 8.0 (b). The Ag^+ ions were added into the assembled solution at pH of 2.5 when the reaction time was 10 mins.
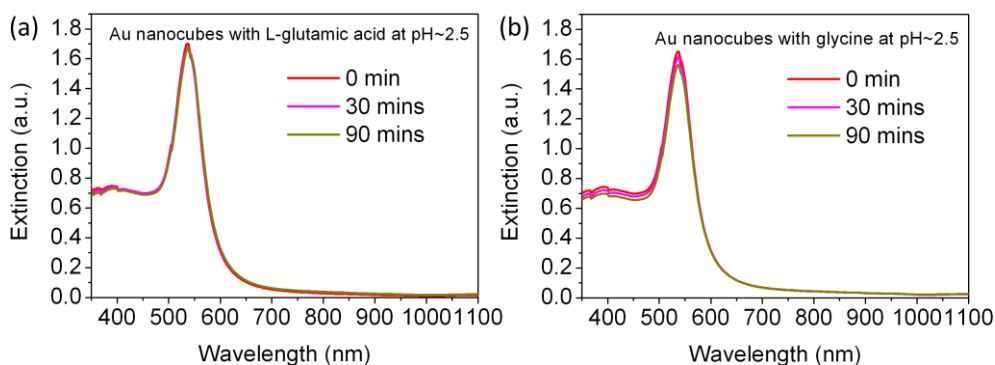

Fig. S2 Extinction spectra of the original Au nanocubes and the products with the assembly reaction time of 30 and 90 mins by using L-glutamic acid (a) and glycine (b) to replace Cys.
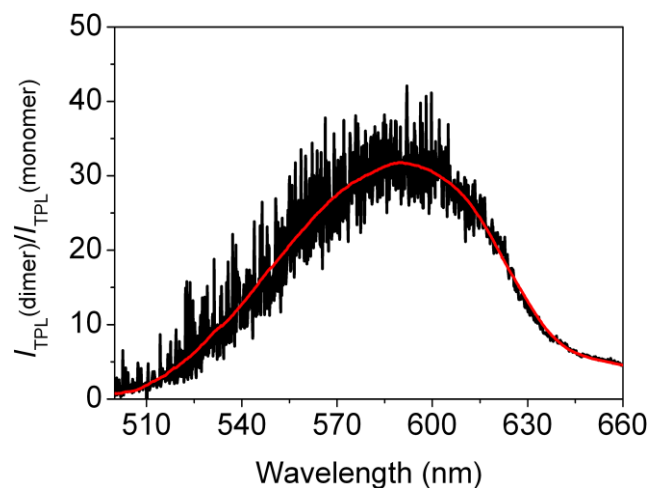
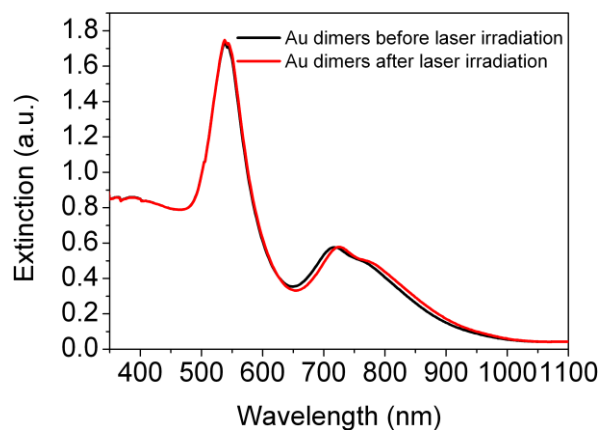**Fig. S3** The TPL intensity ratio of the Au dimers and monomers at the excitation wavelength 710 nm.

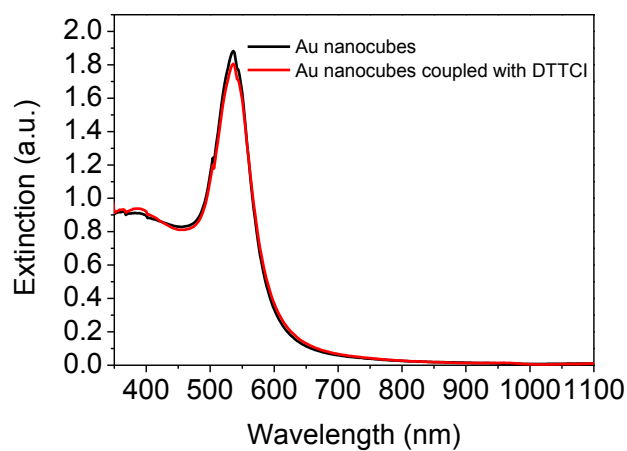**Fig. S4** Extinction spectra of Au nanocube dimers before and after laser irradiation.

Fig. S5 Extinction spectra of Au nanocubes were before and after coupled with DTTCI.
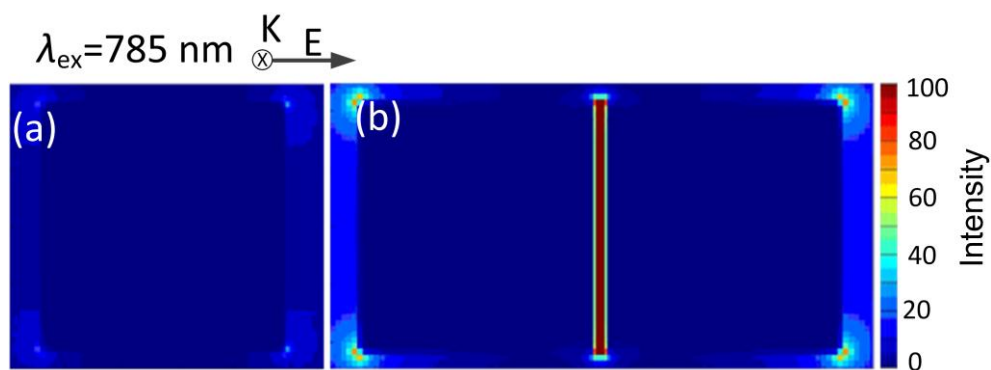
Fig. S6 FDTD simulations of electric field distribution of one Au nanocube monomer (a) and dimer (b) for central cross section at wavelengths of 785 nm. The FDTD simulations were performed using FDTD Solutions 6.5, which was developed by Lumerical Solutions, Inc. The dielectric constants of gold were taken from the Handbook of optical constants of solids of Palik.[1] In the calculations, the mesh around the Au nanostructure was 1 nm * 1 nm * 1 nm and in the gap the mesh was 0.4 nm * 1 nm *1 nm where 0.4 nm is along the gap. Because Au nanocubes were dispersed in aqueous solutions, the refractive index of the medium was taken to be 1.333.

References

1. E. D. Palik, Handbook of Optical Constants of Solids. Academic Press; San Diego, Calif, 1998,(3).