Supporting information

Ligand exchange of $Au_{25}SG_{18}$ leading to functionalized gold clusters: Spectroscopy, kinetics and luminescence

E. S. Shibu[Ŧ], M. A. Habeeb Muhammed[Ŧ], T. Tsukuda[†] and T. Pradeep[Ŧ*]

[Ŧ] *DST Unit on Nanoscience (DST UNS), Department of Chemistry and Sophisticated Analytical Instrument Facility, Indian Institute of Technology, Madras, Chennai 600 036, India.*

[†] *Institute for Molecular Science, Myodaiji, Okazaki 444-8585, Japan.*

* Corresponding author. Fax: + 91-44 2257-0545. E-mail: pradeep@iitm.ac.in.

Supporting Information S1

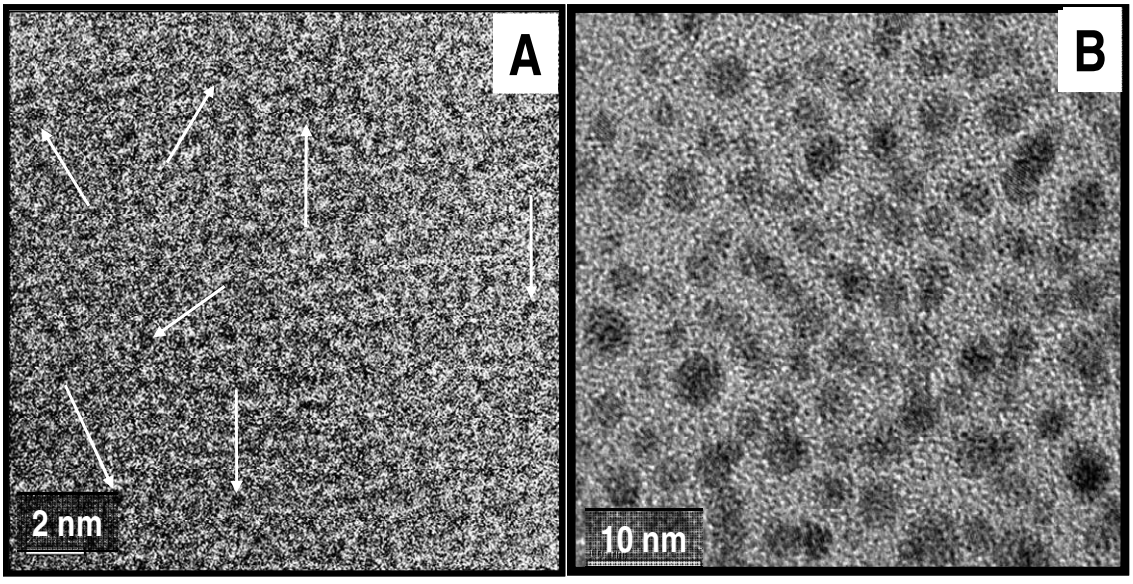


Figure S1. (A) TEM image of $Au_{25}SG_{18}$. (B) The systematic conversion of clusters into bigger nanoparticles upon the irradiation of the electron beam, when a grid with larger particle density was irradiated.

Supporting Information S2

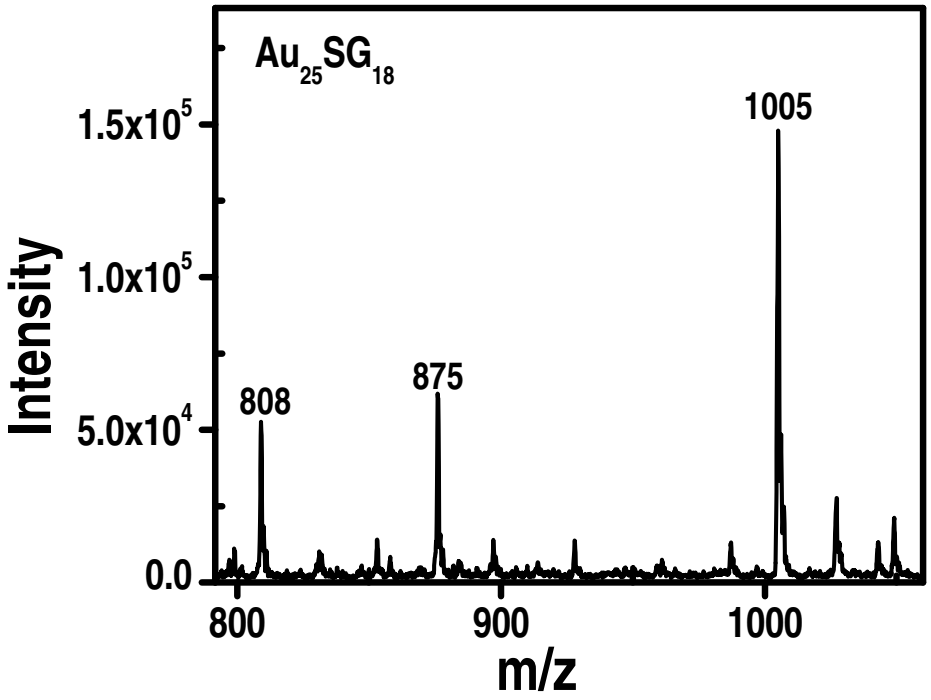
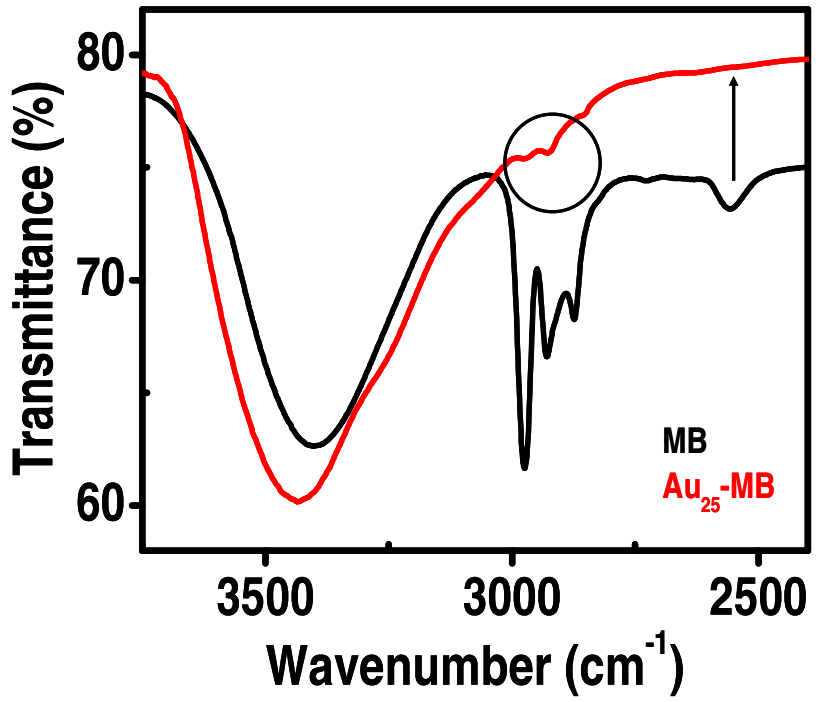


Figure S2. ESI mass spectrum of $Au_{25}SG_{18}$, which gives characteristic peaks at m/z 808 and 1005 due to $[Au(SG)_2\text{-}H]^{-1}$ and $[Au_2(SG)_2\text{-}H]^{-1}$, respectively.

Supporting Information S3



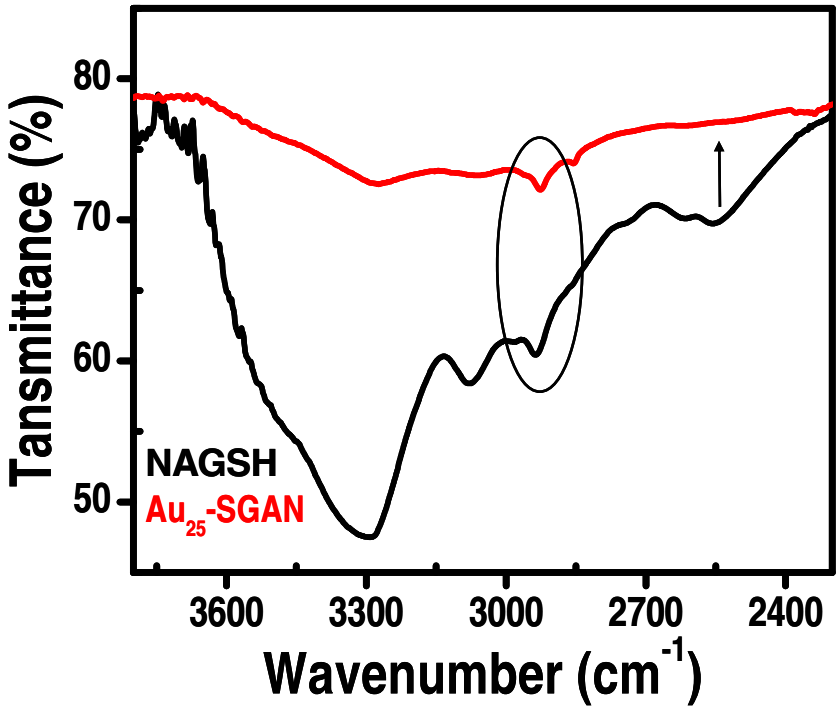


Figure S3. Expanded FT-IR of (A) MB and $Au_{25}SG_{18}$; and (B) NAGSH and Au_{25}-SGAN. Note the disappearance of the thiol peaks.

Supporting Information S4

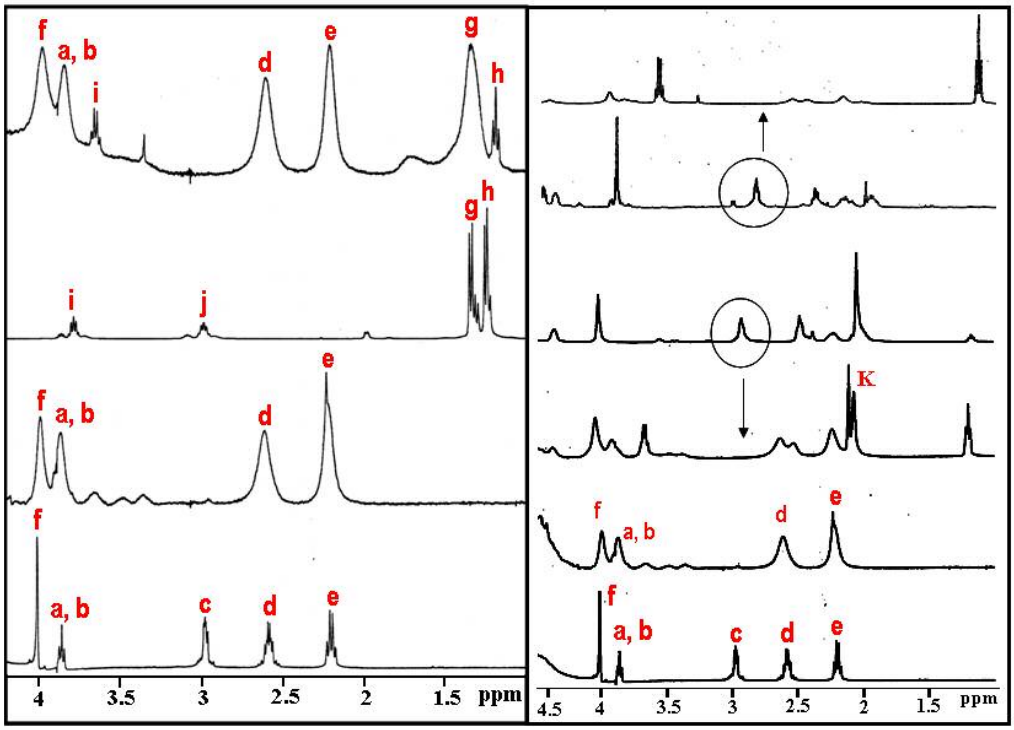
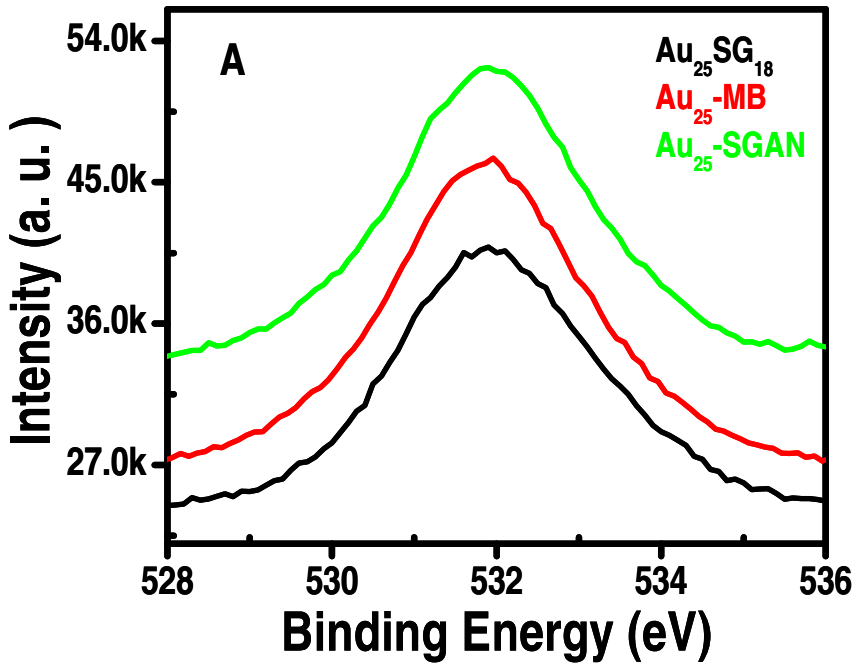


Figure S4. (A) Expanded ^{1}H NMR of (A) GSH, $Au_{25}SG_{18}$, MB and Au_{25}-MB; and (B) GSH, $Au_{25}SG_{18}$, NAGSH, Au_{25}-SGAN, NFGSH and Au_{25}-SGFN.

Supporting Information S5



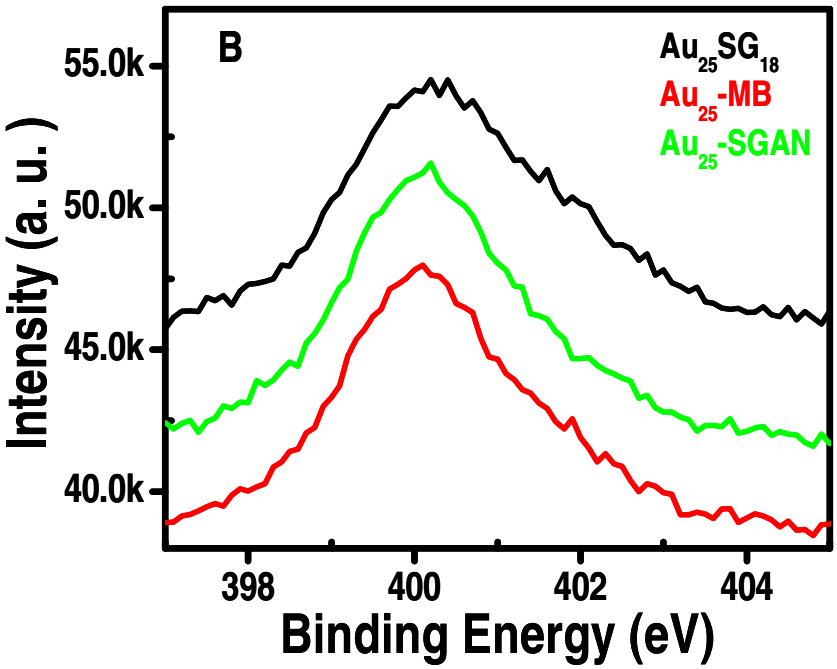


Figure S5. O1s (A) and N1s (B) core level photoelectron spectra of $Au_{25}SG_{18}$, Au_{25}-MB and Au_{25}-SGAN respectively.

Supporting Information (Table 1)

Elemental analysis data of $Au_{25}SG_{18}$, Au_{25}-MB and Au_{25}-SGAN

$[Au_{25}SG_{18}]$

Elements	Calculated values	Expected values
N	7.19	7.23
C	20.28	20.67
H	3.34	2.77
S	5.96	5.52
Total	36.77	36.20

$[Au_{25}(MB)_5(SG)_{13}]$

Elements	Calculated values	Expected values
N	5.23	5.78
C	18.54	18.11
H	3.21	2.69
S	5.40	6.11
Total	32.38	32.69

For compositions mentioned above and those listed below, the expected values are somewhat different.

For $[Au_{25}(MB)_4(SG)_{14}]$- Total C,H,N,S % =34.22

For $[Au_{25}(MB)_6(SG)_{12}]$- Total C,H,N,S % =33.09

$[Au_{25}(SGAN)_{15}(SG)_3]$

Elements	Calculated values	Expected values
N	6.29	6.83
C	20.49	22.78
H	3.23	2.89
S	5.32	5.21
Total	35.33	37.71

For composition mentioned above and those listed below, the expected values are somewhat different.

For $[Au_{25}(SGAN)_{13}(SG)_5]$- Total C,H,N,S % =37.53

For $[Au_{25}(SGAN)_{14}(SG)_4]$- Total C,H,N,S % =37.63