

## Supporting information

### Ligand exchange of Au<sub>25</sub>SG<sub>18</sub> leading to functionalized gold clusters: Spectroscopy, kinetics and luminescence

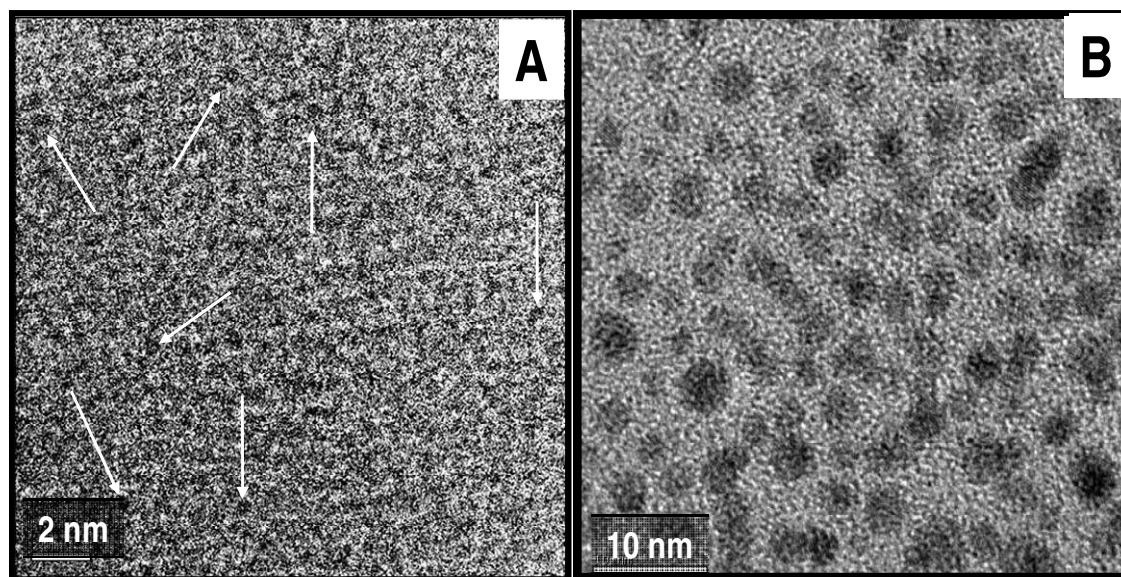
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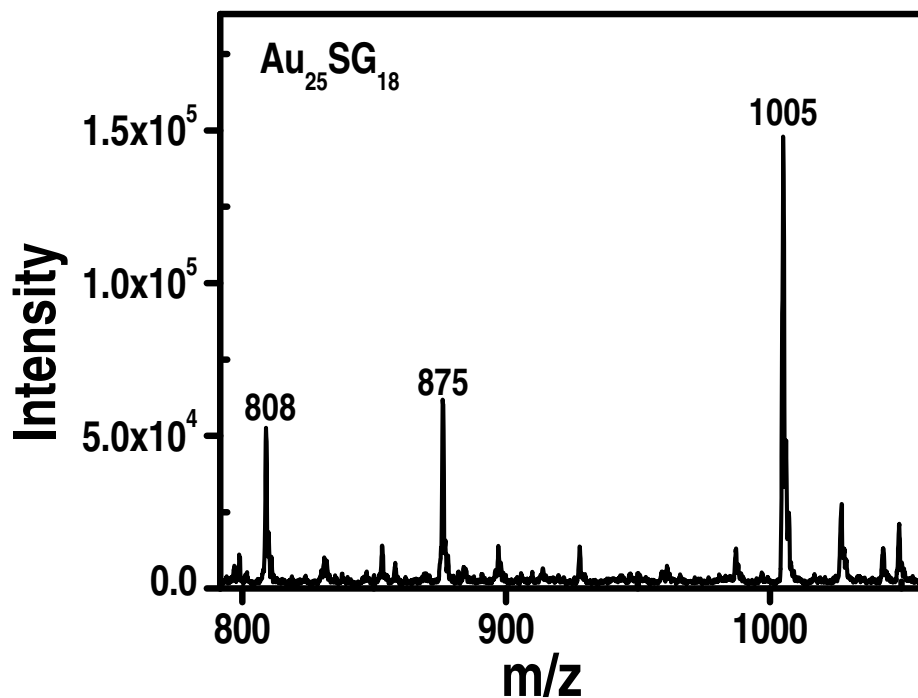
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#### Supporting Information S1



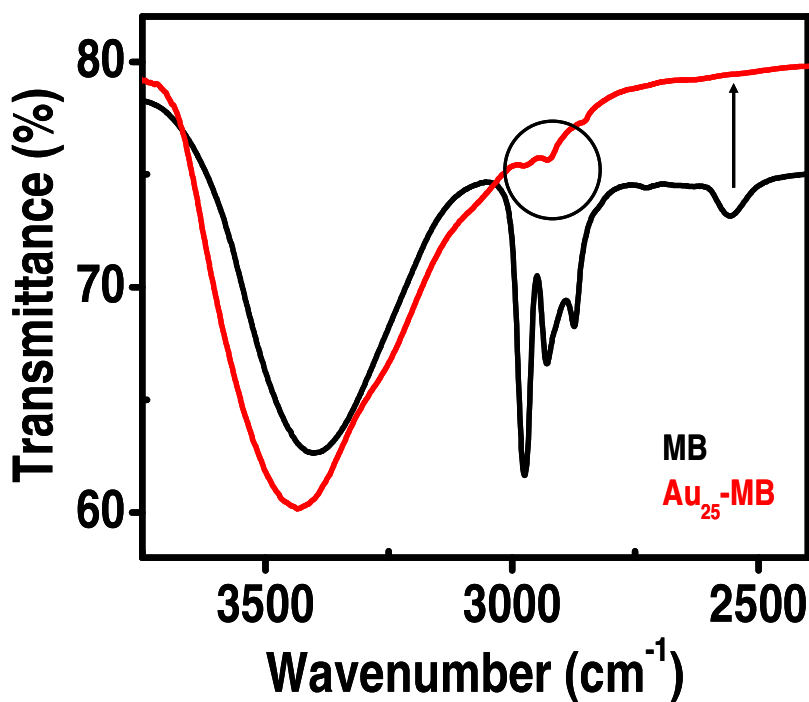
**Figure S1.** (A) TEM image of Au<sub>25</sub>SG<sub>18</sub>. (B) The systematic conversion of clusters into bigger nanoparticles upon the irradiation of the electron beam, when a grid with larger particle density was irradiated.

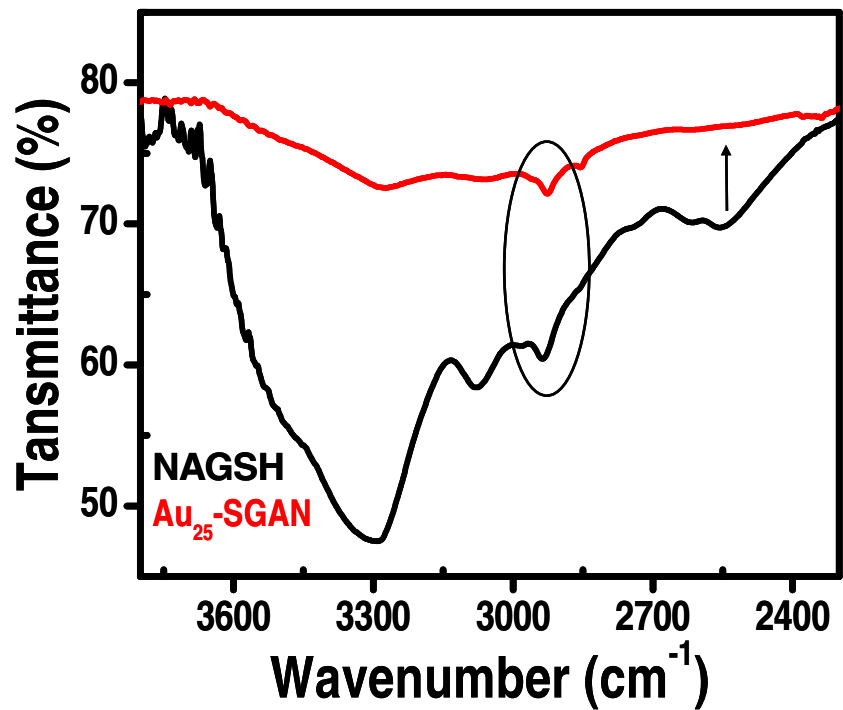
Supporting Information S2



**Figure S2.** ESI mass spectrum of Au<sub>25</sub>SG<sub>18</sub>, which gives characteristic peaks at m/z 808 and 1005 due to [Au(SG)<sub>2</sub>-H]<sup>-1</sup> and [Au<sub>2</sub>(SG)<sub>2</sub>-H]<sup>-1</sup>, respectively.

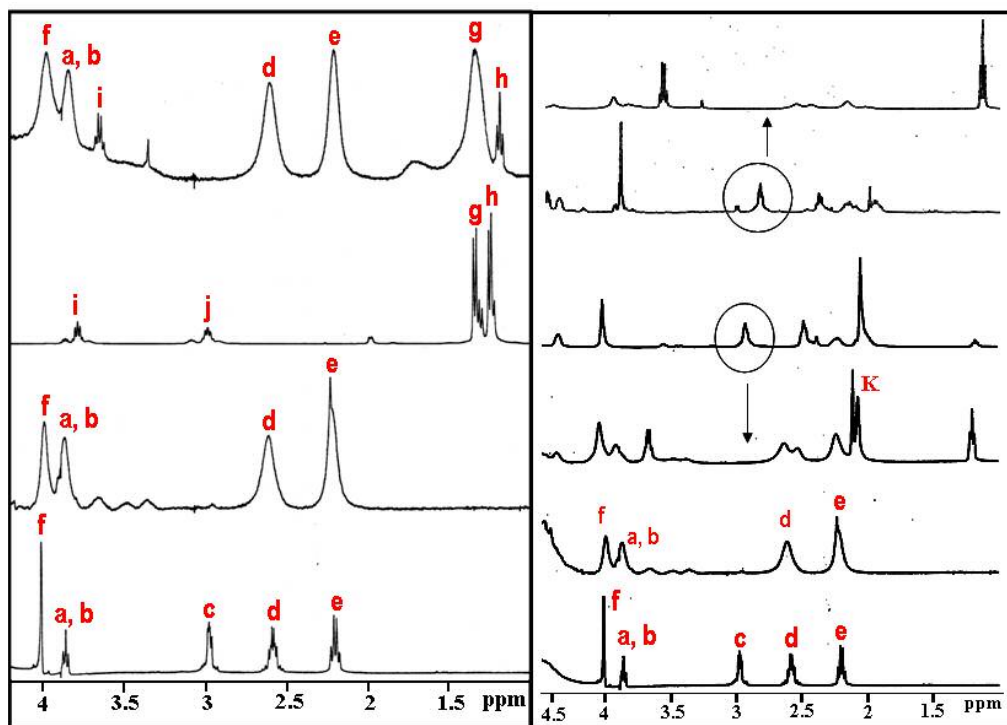
Supporting Information S3





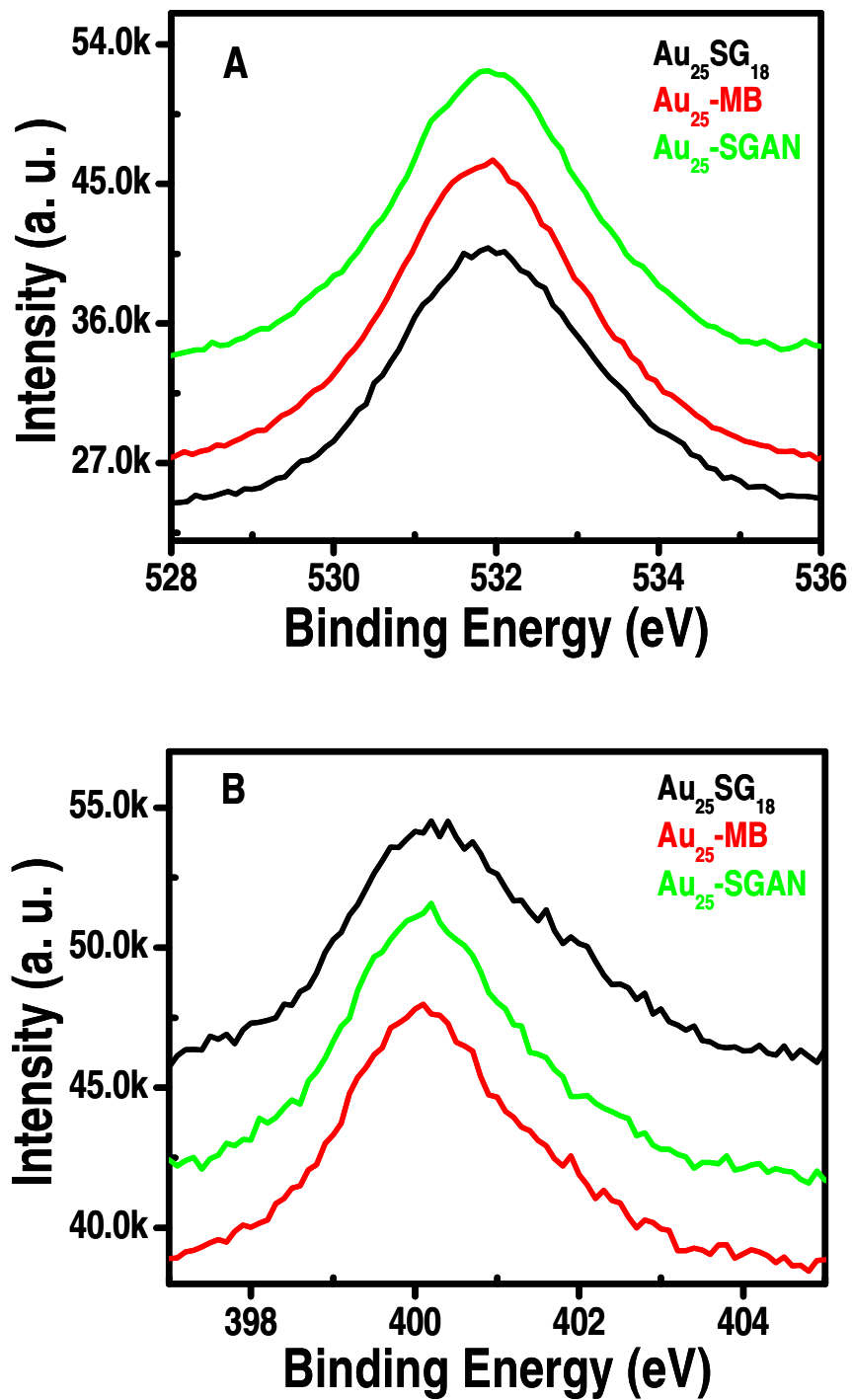
**Figure S3.** Expanded FT-IR of (A) MB and Au<sub>25</sub>SG<sub>18</sub>; and (B) NAGSH and Au<sub>25</sub>-SGAN. Note the disappearance of the thiol peaks.

**Supporting Information S4**



**Figure S4.** (A) Expanded  $^1\text{H}$  NMR of (A) GSH,  $\text{Au}_{25}\text{SG}_{18}$ , MB and  $\text{Au}_{25}\text{-MB}$ ; and (B) GSH,  $\text{Au}_{25}\text{SG}_{18}$ , NAGSH,  $\text{Au}_{25}\text{-SGAN}$ , NFGSH and  $\text{Au}_{25}\text{-SGFN}$ .

Supporting Information S5



**Figure S5.** O1s (A) and N1s (B) core level photoelectron spectra of Au<sub>25</sub>SG<sub>18</sub>, Au<sub>25</sub>-MB and Au<sub>25</sub>-SGAN respectively.

**Supporting Information (Table 1)**

Elemental analysis data of Au<sub>25</sub>SG<sub>18</sub>, Au<sub>25</sub>-MB and Au<sub>25</sub>-SGAN

[Au<sub>25</sub>SG<sub>18</sub>]

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<sub>25</sub>(MB)<sub>5</sub>(SG)<sub>13</sub>]

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

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

$[\text{Au}_{25}(\text{SGAN})_{15}(\text{SG})_3]$

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

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