

# **CHEMISTRY**

---

## **A EUROPEAN JOURNAL**

---

### Supporting Information

© Copyright Wiley-VCH Verlag GmbH & Co. KGaA, 69451 Weinheim, 2009

# **Clusters from Clusters: Bright, NIR Emitting Au<sub>23</sub> from Au<sub>25</sub>- Charecterisation and Applications Including Bio-Labeling**

M. A. Habeeb Muhammed<sup>a</sup>, Pramod Kumar Verma<sup>b</sup>, Samir Kumar Pal<sup>b\*</sup>, R. C. Arun Kumar<sup>c</sup>,  
Soumya Paul<sup>c</sup>, R. V. Omkumar<sup>c\*</sup> and T. Pradeep<sup>a\*</sup>

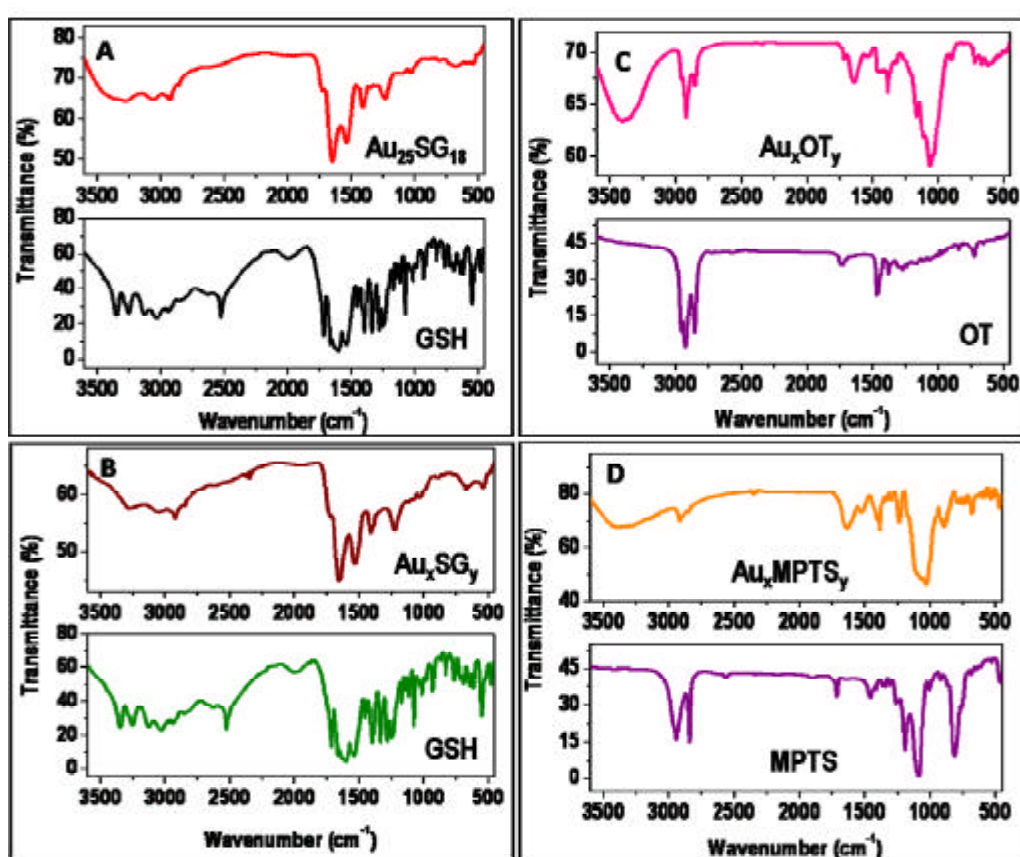
<sup>a</sup>*DST Unit on Nanoscience (DST UNS), Department of Chemistry and Sophisticated Analytical Instrument Facility,  
Indian Institute of Technology Madras, Chennai - 600 036, India*

<sup>b</sup>*Unit for Nanoscience and Technology, Department of Chemical, Biological and Macromolecular Sciences,  
Satyendra Nath Bose National Centre for Basic Sciences,  
Block JD, Sector III, Salt Lake, Kolkata 700 098, India.*

<sup>c</sup>*Department of Neurobiology, Rajiv Gandhi Center for Biotechnology Thiruvananthapuram, 624000 India*

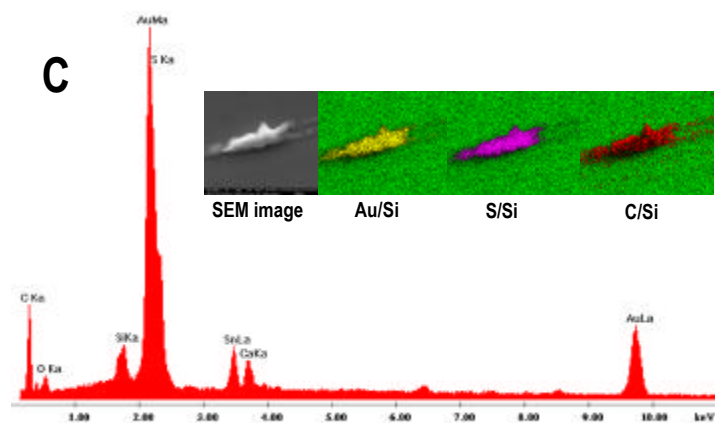
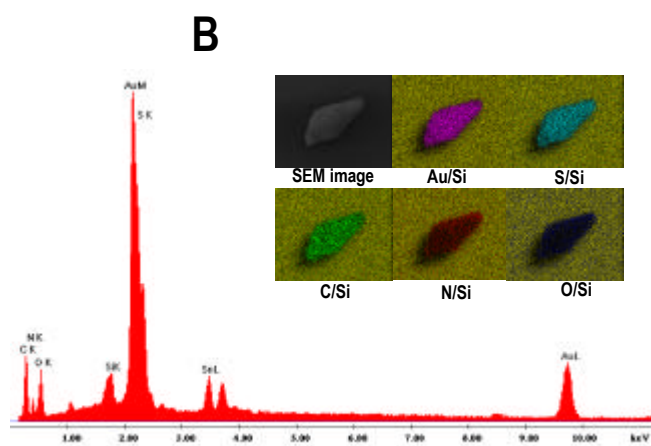
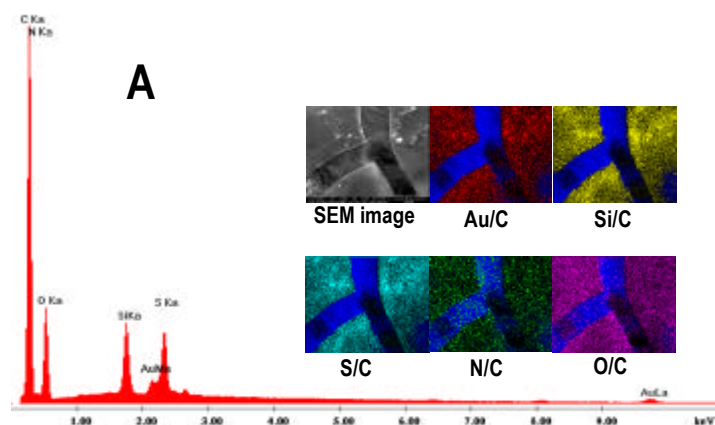
*\*E-mail: [pradeep@iitm.ac.in](mailto:pradeep@iitm.ac.in)*

## Supporting information 1



**Figure S1.** Comparison of the FT-IR spectra of the clusters and the corresponding ligands used for etching, with the parent  $\text{Au}_{25}\text{SG}_{18}$ .

## Supporting information 2

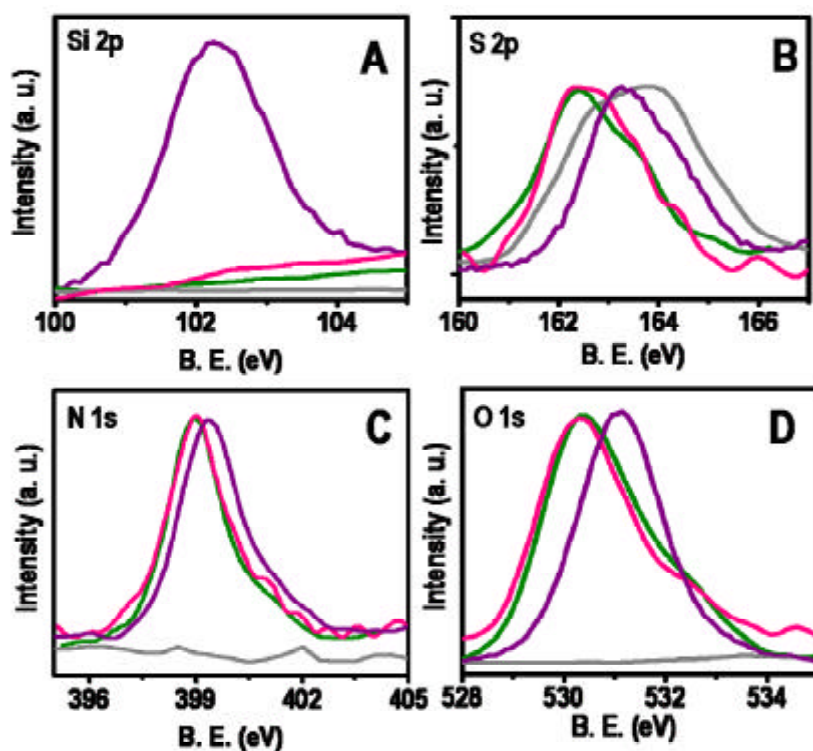




Sample	Element	% of element (Experimental)	% of element (Calculated)	Molecular formula
$\text{Au}_x\text{MPTS}_y$	N	03.85	03.68	$\text{Au}_{22}(\text{MPTS})_{10}(\text{SG})_7$
	C	15.29	15.03	
	H	02.71	02.62	
	S	06.31	06.81	
$\text{Au}_x\text{SG}_x$	N	07.75	07.53	$\text{Au}_{23}\text{SG}_{18}$
	C	20.68	21.52	
	H	03.45	02.87	
	S	05.48	05.74	
$\text{Au}_x\text{OT}_y$	N	00.00	00.00	$\text{Au}_{33}\text{OT}_{22}$
	C	22.01	21.78	
	H	04.15	03.86	
	S	07.18	07.26	

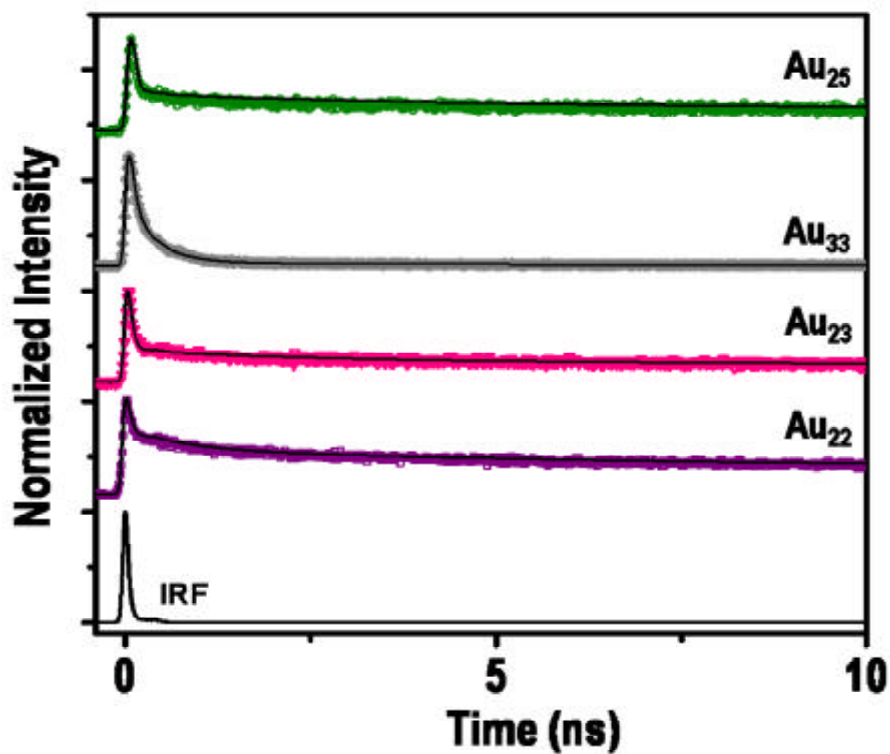
**Figure S2.** EDAX spectra and corresponding elemental mappings of A)  $\text{Au}_x\text{MPTS}_y$ , B)  $\text{Au}_x\text{SG}_y$  and C)  $\text{Au}_x\text{OT}_y$ . Element C in data set A is from the carbon tape used as the substrate. The elemental mappings are overlayed with carbon for clarity. Elements Si, Sn and O in B and C in data sets B and C are from the conducting glass surface used as the substrate. The elemental mappings are overlayed with silicon for clarity. Table shows CHNS elemental analysis data of the three clusters.

### Supporting information 3



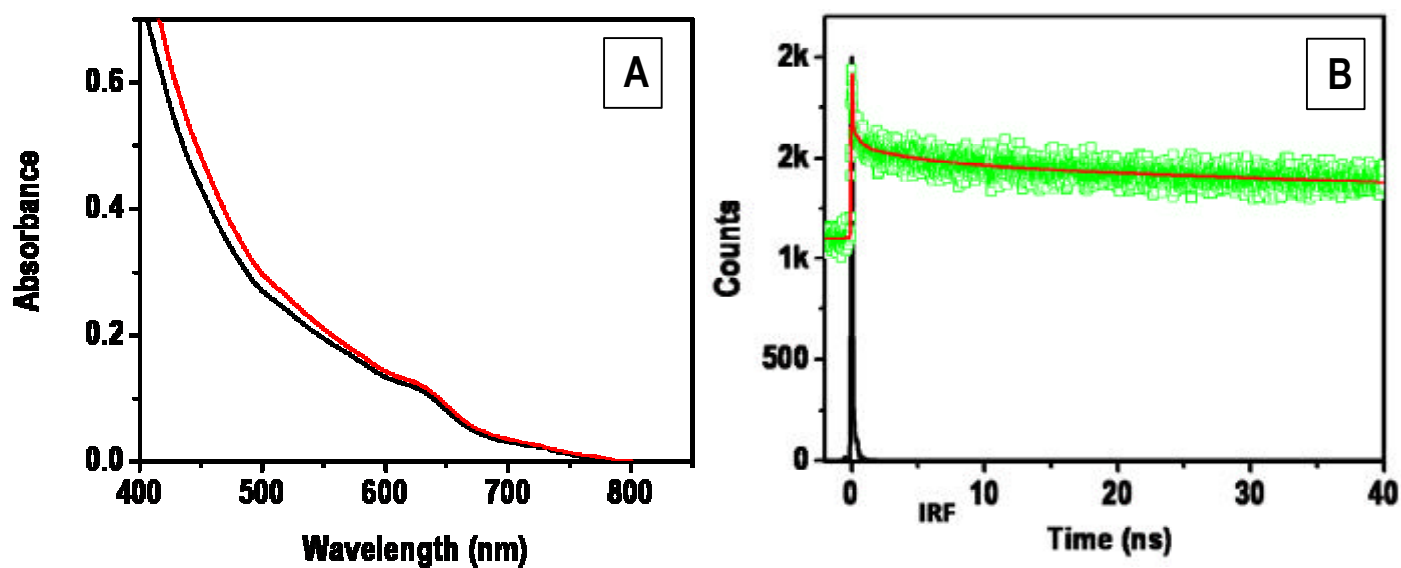
**Figure S3.** A) Comparison of XPS spectra due to the core level photoemission from Si2p, S2p , N1s and O1s of Au<sub>33</sub> (grey trace), Au<sub>25</sub> (green trace), Au<sub>23</sub> (pink trace) and Au<sub>22</sub> (purple trace).

#### Supporting information 4



**Figure S4.** Fluorescence decay pattern of Au<sub>25</sub>, Au<sub>33</sub>, Au<sub>23</sub>, and Au<sub>22</sub> collected at 630 nm.

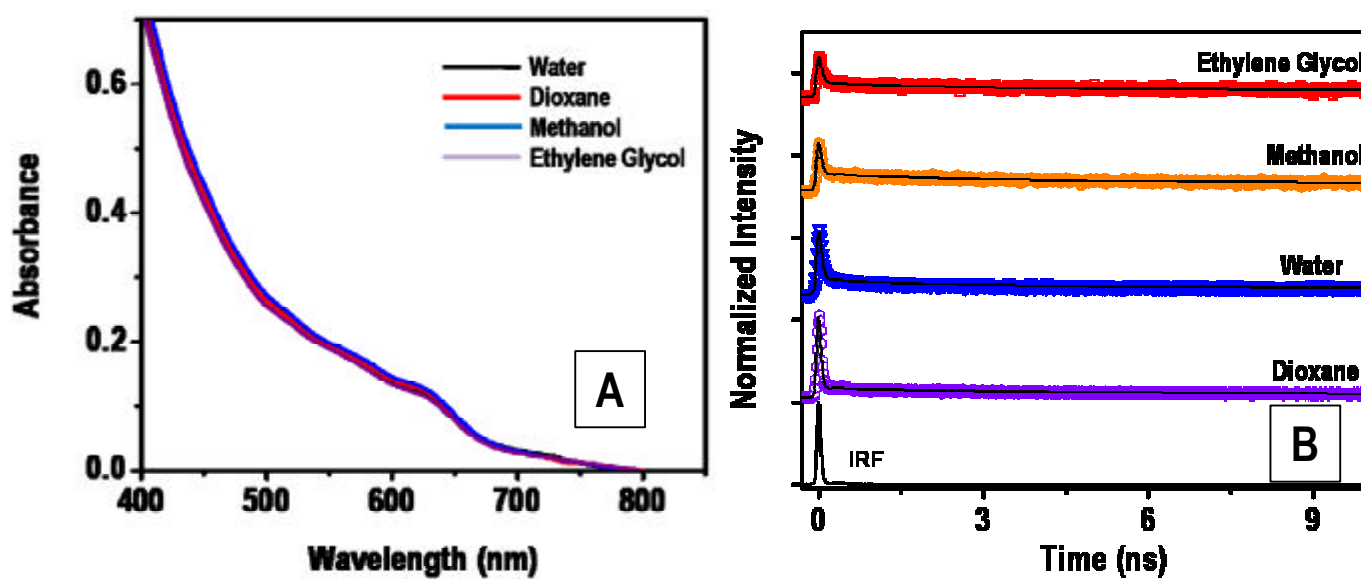
#### Supporting information 5



Solvent	$t_1$ (ps)	%	$t_2$ (ns)	%	$t_3$ (ns)	%
Toluene	34	82.8	4.11	4.3	80.35	12.9
Water	39	92.4	2.41	3.6	68.55	3.9

**Figure S5.** A) Optical absorption spectra of Au<sub>23</sub> before (red trace) and after (black trace) phase transfer. B) Fluorescence decay of Au<sub>23</sub> after phase transfer. Table tabulates the life time values of the cluster before and after phase transfer.

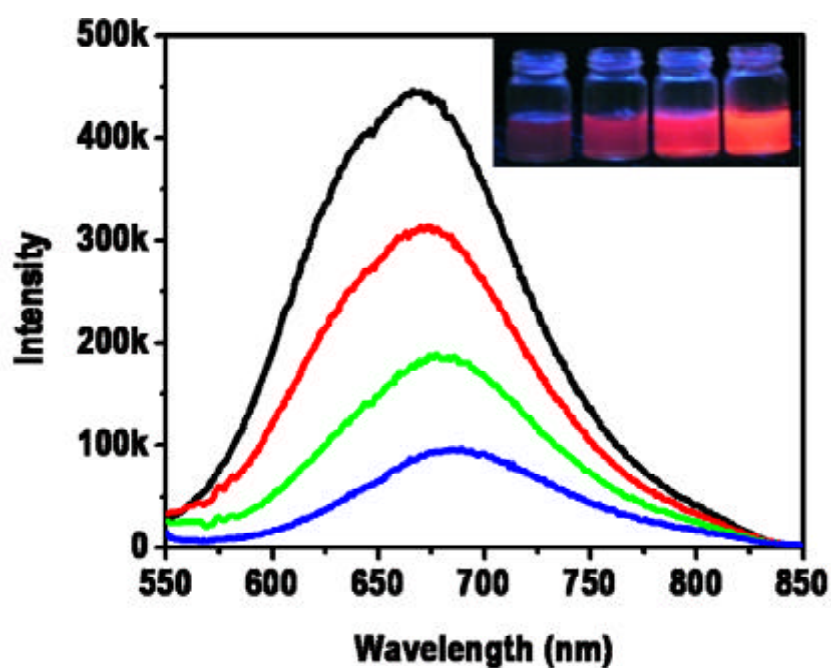
## Supporting information 6



Solvent	$t_1$ (ps)	%	$t_2$ (ns)	%	$t_3$ (ns)	%
Ethylene Glycol	47	86.5	2.67	5.5	70.06	7.9
Methanol	36	87.6	3.27	5.8	62.91	6.6
Water	39	92.4	2.41	3.6	68.55	3.9
Dioxane	16	98.0	5.07	1.1	31.63	0.9

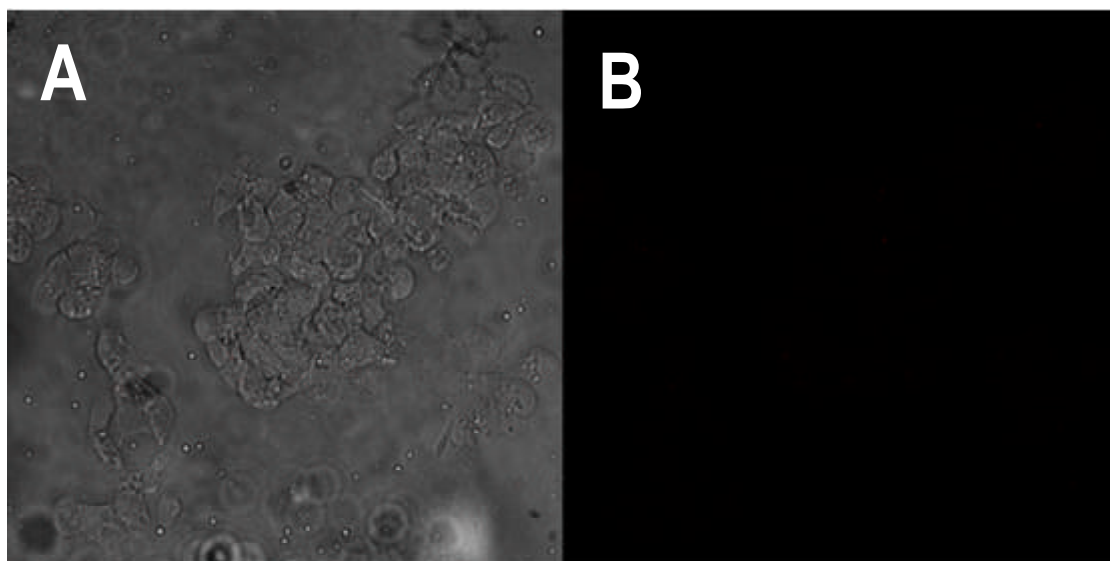
**Figure S6.** A) Optical absorption spectra of Au<sub>23</sub> in dioxane, water, methanol and ethylene glycol. B) Fluorescence decay of Au collected at 630 nm in various solvents. Table tabulates the life time of the cluster in various solvents.

## Supporting information 7



**Figure S7.** Plot of fluorescence intensity of Au<sub>23</sub> cluster in water-DMSO mixture starting from pure water (blue line) to 1:1 (green line), 1:2 (red line) and 1:3 (black trace) water-DMSO mixtures. Inset shows the photographs of the corresponding solutions under UV light irradiation.

## Supporting information 8



**Figure S8.** Bright field (A) and fluorescence (B) images of HepG2 cells stained with unconjugated Au<sub>23</sub> clusters. No fluorescence was observed from the cells after washing.