Electronic Supplementary Information (ESI)

Experimental and computational insights into luminescence in atomically precise bimetallic $Au_{6-n}Cu_n(MPA)_5$ (n=0-2) clusters

Aarti Devi[1], Harshita Seksaria[1], Dipankar Bain[1], Sarita Kolay[2], Rashi[1], Abir De Sarkar[1] and Amitava Patra[1,2]*

[1]Institute of Nano Science and Technology, Knowledge City, Sector 81, Mohali 140306, India

[2]School of Materials Sciences, Indian Association for the Cultivation of Science, Kolkata 700032, India

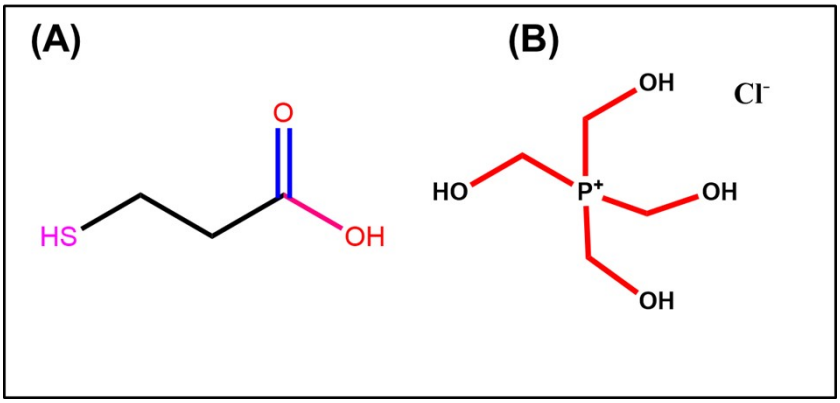


Fig S1: Molecular structures of (A) MPA and (B) THPC

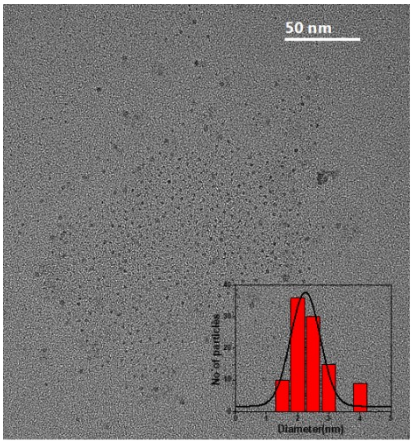


Fig. S2: TEM image of AuCu-1 NCs. Inset shows the corresponding particle size distribution.

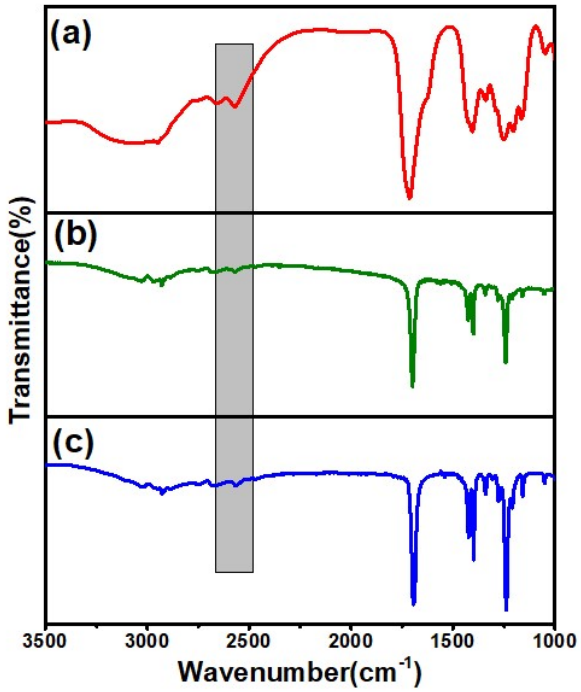


Fig. S3: FTIR Spectra of (a) MPA Ligand (b) Au NCs (c) AuCu-2 NCs

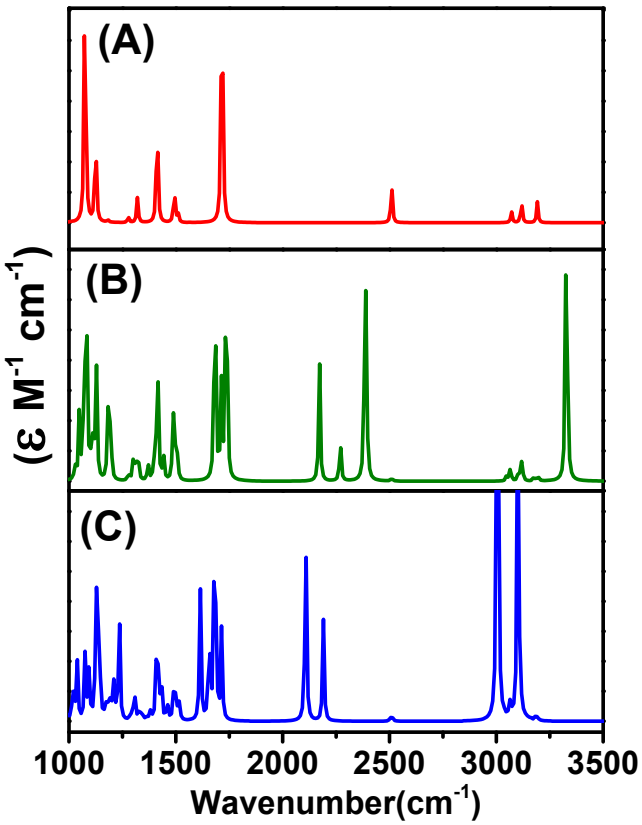


Fig. S4: Theoretical predicted IR Spectra of (A) MPA Ligand (B) Au NCs, and (C) AuCu-2 NCs.

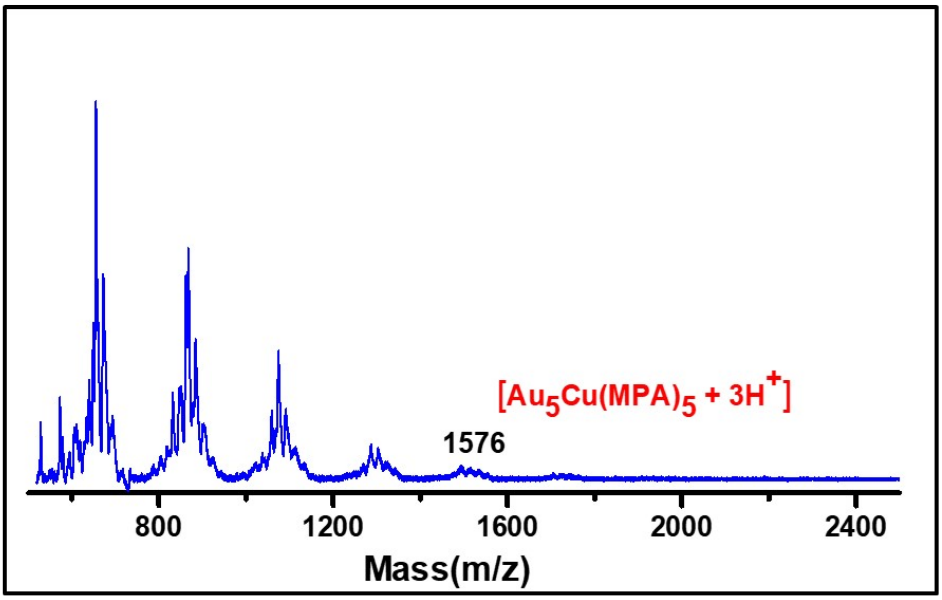


Fig. S5: MALDI-TOF analysis of AuCu-1 NCs.

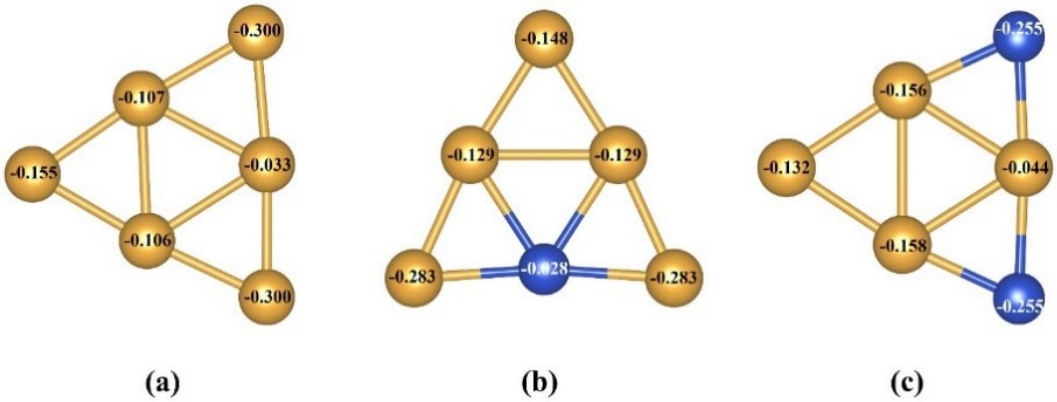
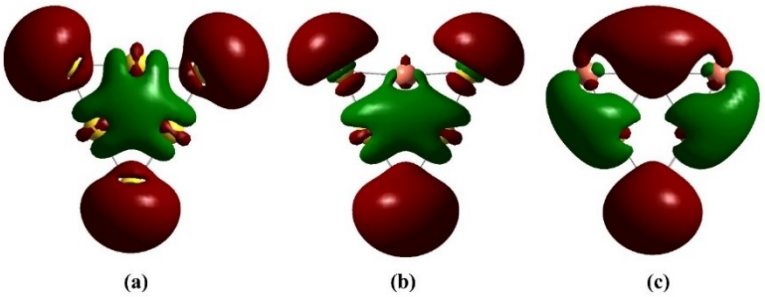


Fig. S6: Electrophilic Fukui functions of (a) Au_6, (b) Au_5Cu_1, and (c) Au_4Cu_2 clusters



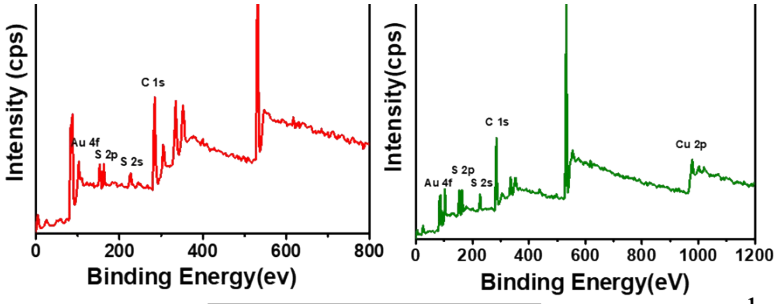


Fig. S7: The lowest-energy unoccupied molecular orbitals (LUMO) of (a) Au_6, (b) Au_5Cu_1, and (c) Au_4Cu_2 clusters (maroon & green colors represent negative and positive charge density)

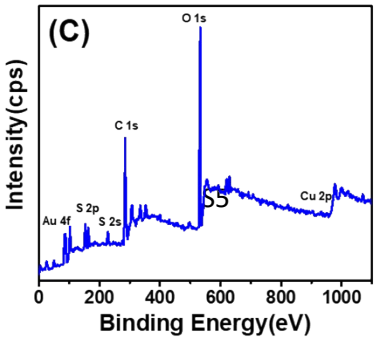


Fig. S8: XPS survey spectra of (A) Au NCs and (B) AuCu-1 NCs (C) AuCu-2 NCs

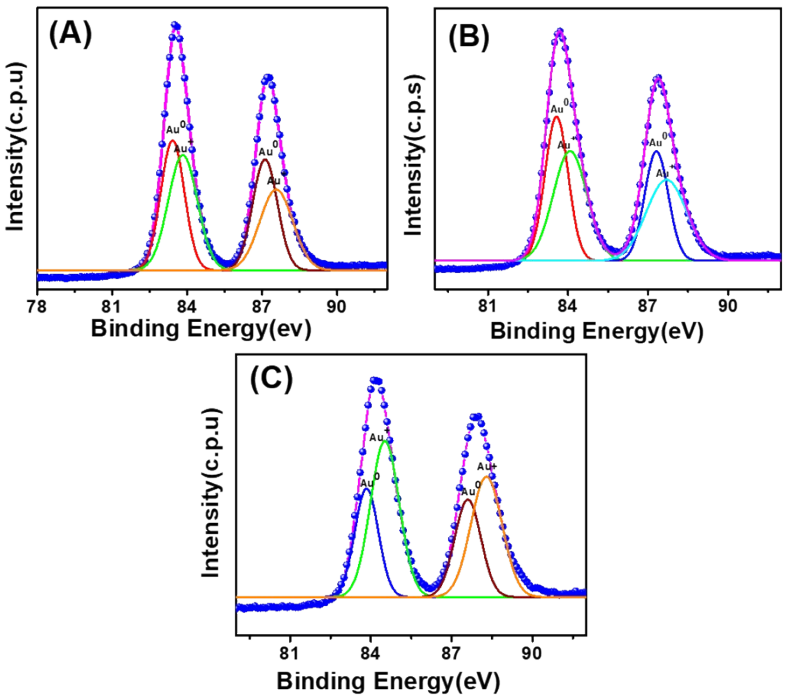


Fig. S9: XPS spectra of Au 4f of (A)Au NCs (B) AuCu-1 NCs (C) AuCu-2 NCs

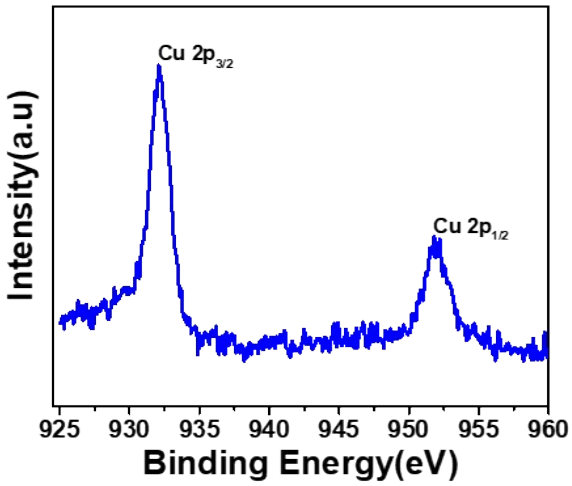


Fig. S10: XPS spectrum of Cu 2p in AuCu-2 NCs

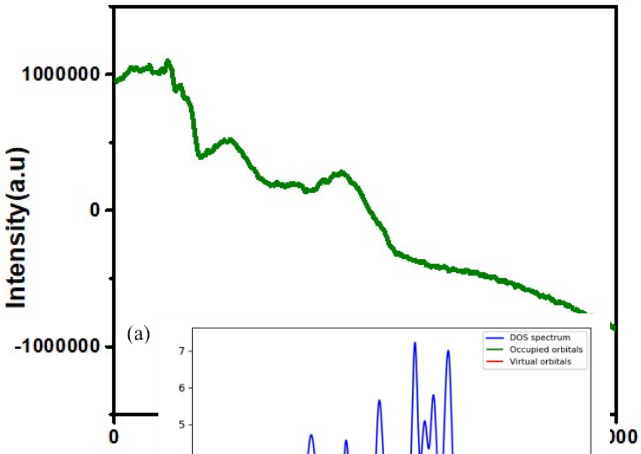


Fig. S11: EPR spectrum of AuCu-2 NCs.

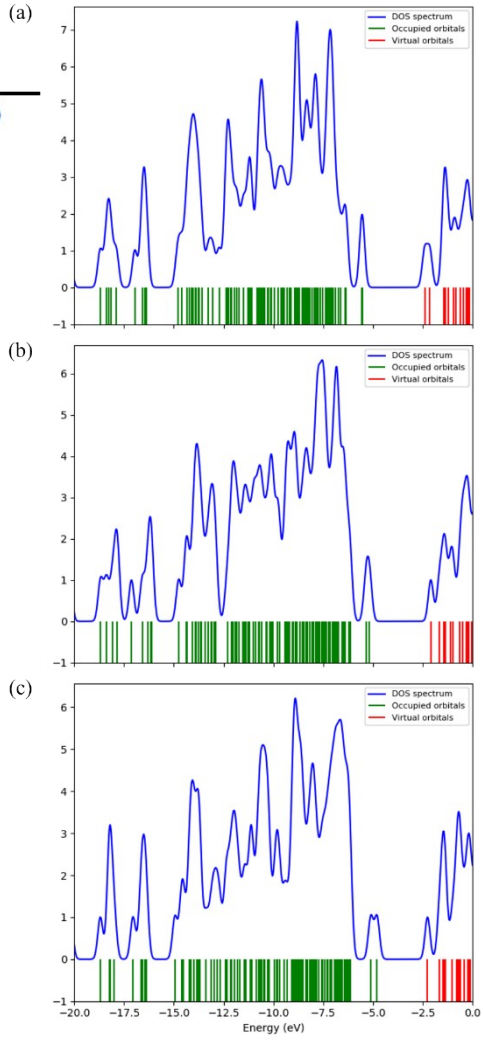


Fig. S12: DOS plot for (a) Au, (b) AuCu-1, and (c) AuCu-2 NCs

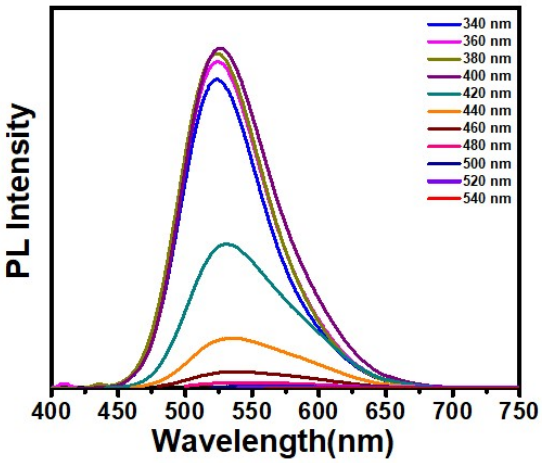


Fig. S13: Excitation-dependent PL of Au NCs.

Table S1: XPS Studies of Au 4f in Au NCs and AuCu NCs.

Systems	**Au $4f_{7/2}$ B.E (eV)**	**Au$4f_{5/2}$ B.E (eV)**	**Shift in comparison with Au NCs(eV)**
Au NCs	83.51	87.25	-
AuCu-1 NCs	83.69	87.38	0.18
AuCu-2 NCs	84.21	87.91	0.70

Table S2: Excitation energy and oscillator strength for the first six singlet excitations for Au and AuCu-2 NCs

Nanocomposite	**Excitation State**	**Energy (eV)**	**Oscillator strength**
Au NC	S1	2.81	0.0477
	S2	2.94	0.0575
	S3	3.13	396.10
	S4	3.24	382.60
	S5	3.79	327.09
	S6	3.88	319.67
AuCu-2 NC	S1	2.16	0.0282
	S2	2.56	0.0445
	S3	2.88	0.1742
	S4	3.09	0.0168
	S5	3.16	0.1519
	S6	3.46	0.0156