

Electronic Supplementary Information (ESI)

**Experimental and computational insights into luminescence in
atomically precise bimetallic $\text{Au}_{6-n}\text{Cu}_n(\text{MPA})_5$ ($n=0-2$) clusters**

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Contents		Page No.
Fig. S1	MPA and THPC structure	S3
Fig. S2	TEM image of AuCu-1 NCs with particle size distribution.	S3
Fig. S3	FTIR spectra of MPA ligand, Au NCs, and AuCu-2 NCs.	S4
Fig. S4	Theoretical predicted FTIR Spectra of MPA ligand, Au NCs and AuCu-2 NCs	S4
Fig. S5	MALDI-TOF analysis of AuCu-1 NCs.	S5
Fig. S6	Electrophilic Fukui functions of Au_6 , Au_5Cu_1 , and Au_4Cu_2 clusters	S5
Fig. S7	The lowest-energy unoccupied molecular orbitals (LUMO) of Au_6 , Au_5Cu_1 , and Au_4Cu_2 clusters	S6
Fig. S8	XPS survey spectra of Au NCs and AuCu(1-2) NCs	S6
Fig. S9	XPS spectra of Au 4f of Au NCs and AuCu(1-2) NCs	S7
Fig. S10	XPS spectra of Cu 2p in AuCu-2 NCs	S7
Fig. S11	EPR Spectrum of AuCu-2 NCs.	S8
Fig. S12	DOS plot for (a) Au, (b) AuCu-1, and (c) AuCu-2 NCs	S8
Fig. S13	Excitation dependent PL of Au NCs	S9
Table S1	XPS Studies of Au 4f in Au NCs and AuCu (1-2) NCs.	S9
Table S2	Excitation energy and oscillator strength for the first six singlet excitations for Au and AuCu-2 NCs	S10

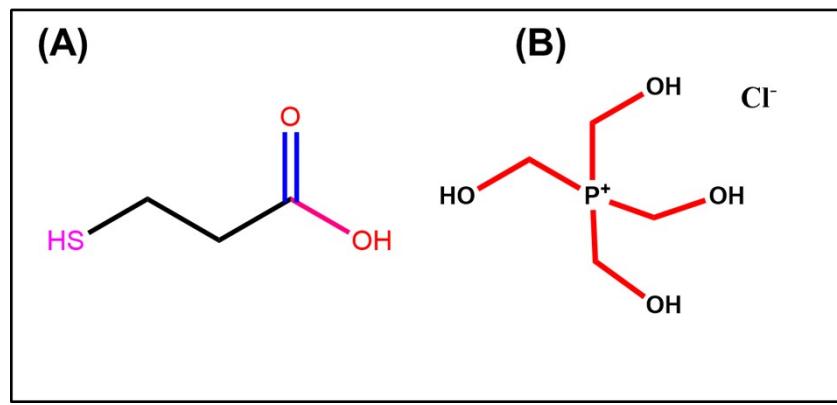


Fig S1: Molecular structures of (A) MPA and (B) THPC

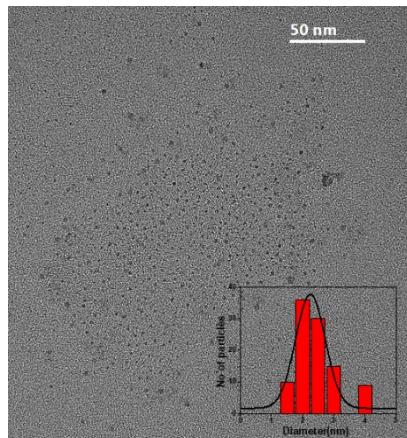


Fig. S2: TEM image of AuCu-1 NCs. Inset shows the corresponding particle size distribution.

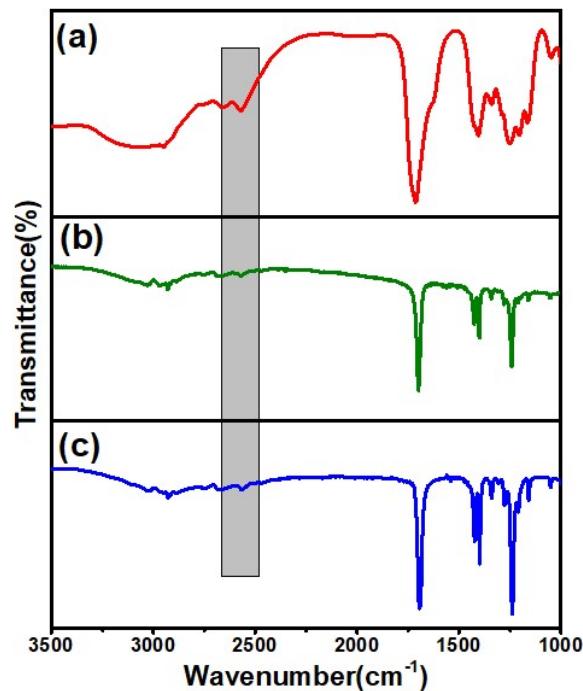


Fig. S3: FTIR Spectra of (a) MPA Ligand (b) Au NCs (c) AuCu-2 NCs

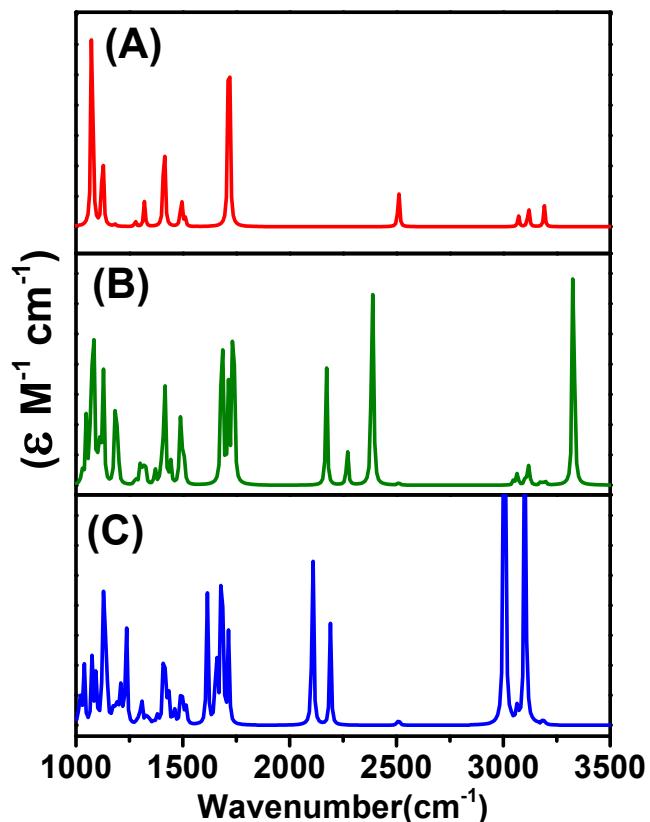


Fig. S4: Theoretical predicted IR Spectra of (A) MPA Ligand (B) Au NCs, and (C) AuCu-2 NCs.

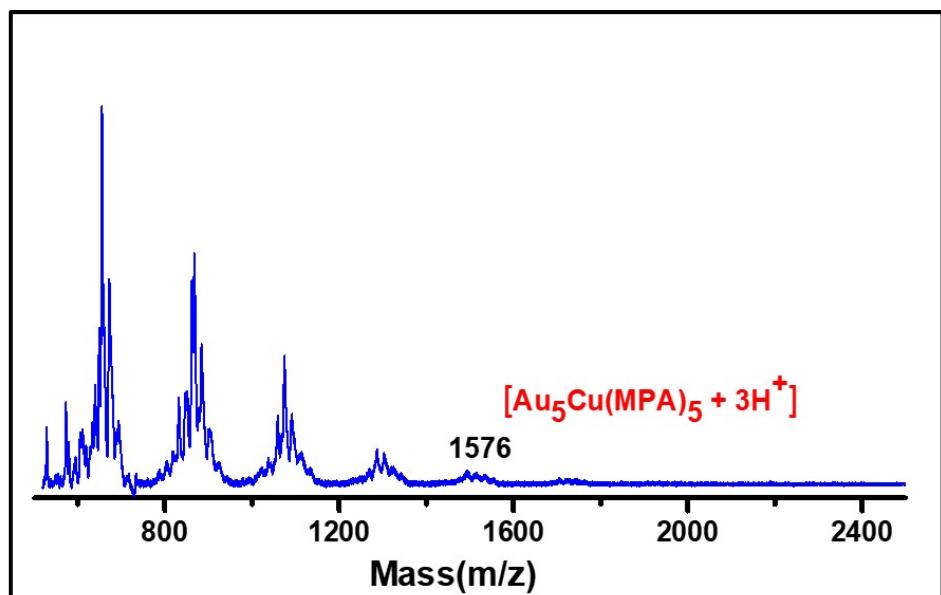


Fig. S5: MALDI-TOF analysis of AuCu-1 NCs.

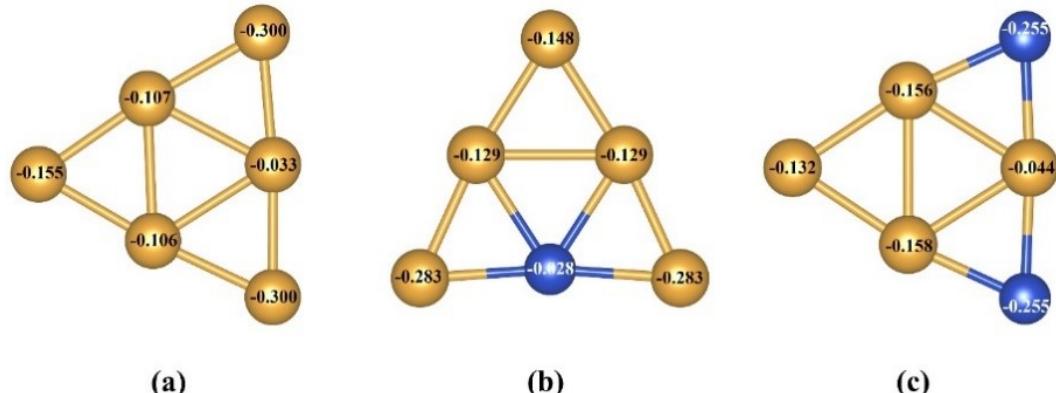


Fig. S6: Electrophilic Fukui functions of (a) Au_6 , (b) Au_5Cu_1 , and (c) Au_4Cu_2 clusters

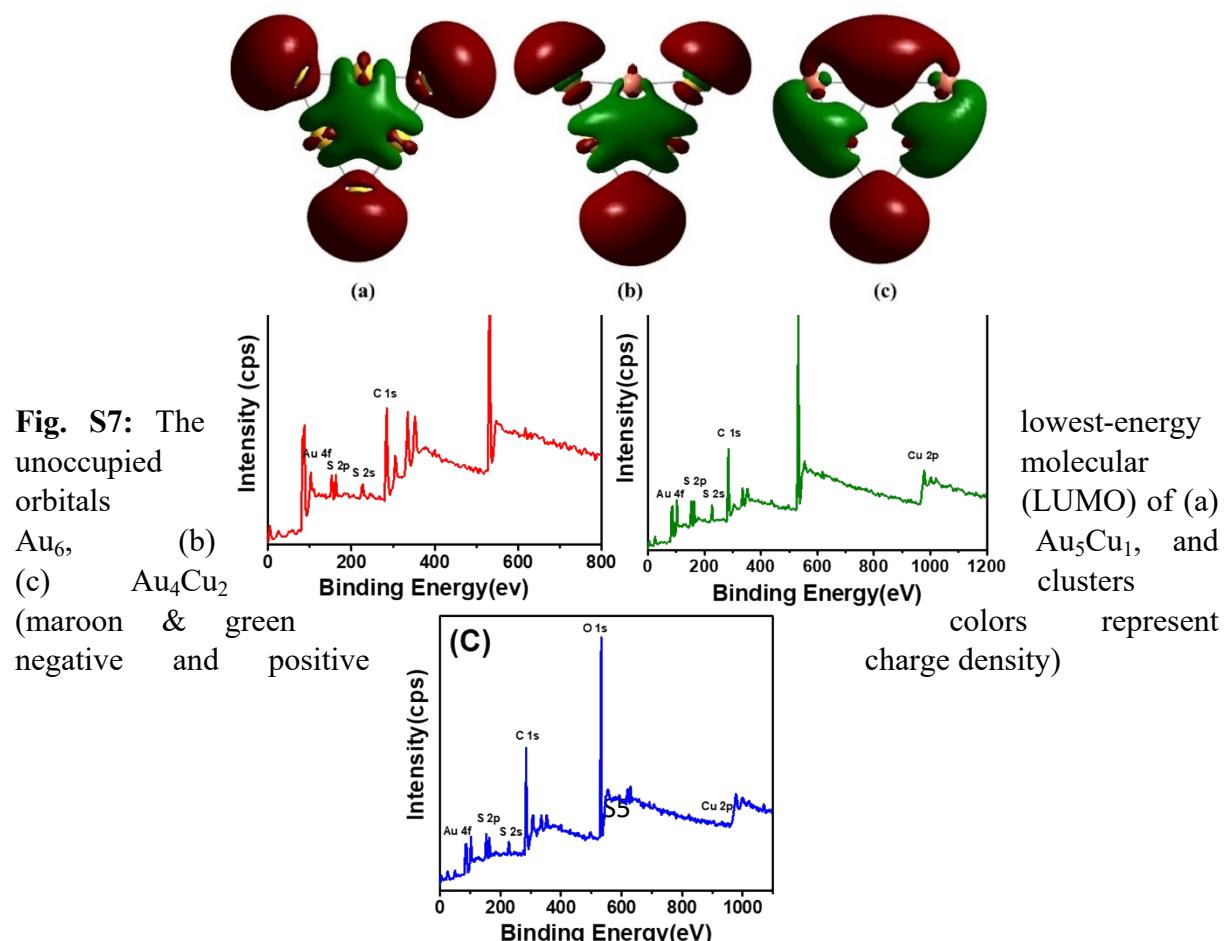


Fig. S7: The unoccupied orbitals
 (a) Au_6 , (b)
 (c) Au_4Cu_2
 (maroon & green
 negative and positive

lowest-energy
 molecular
 (LUMO) of (a)
 Au_5Cu_1 , and
 clusters

colors represent
 charge density)

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

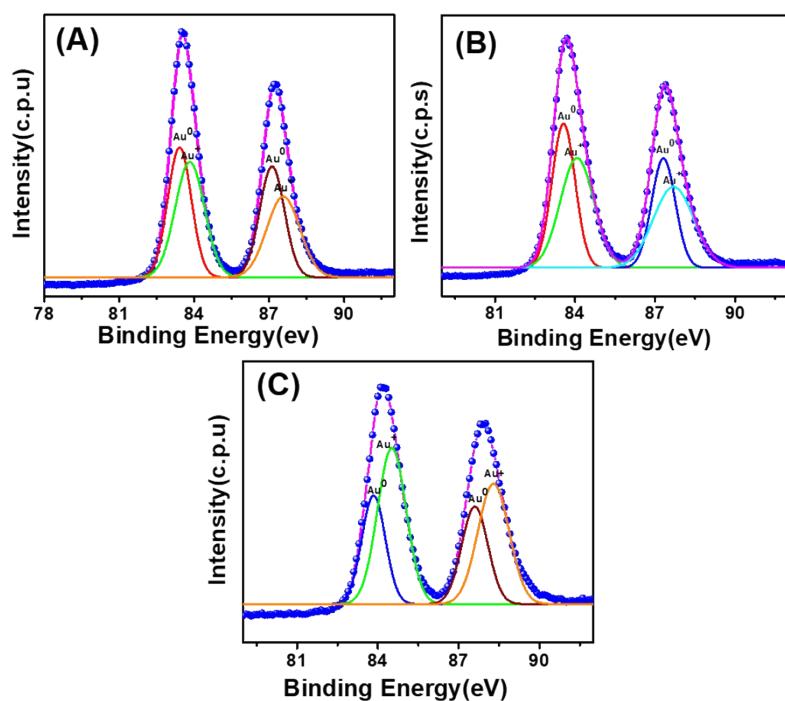


Fig. S9: XPS spectra of Au 4f of (A)Au NCs (B) AuCu-1 NCs (C) AuCu-2 NCs

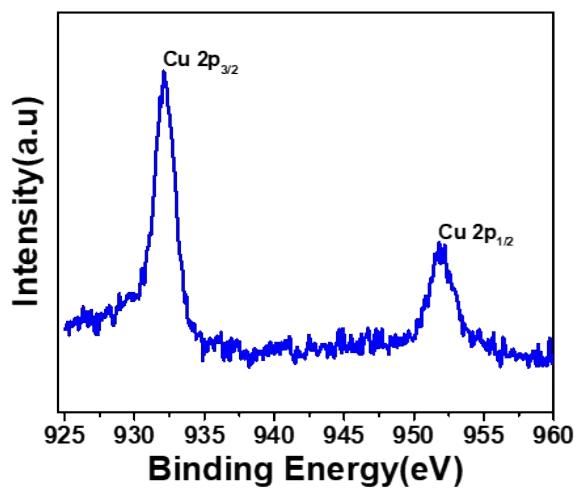


Fig. S10: XPS spectrum of Cu 2p in AuCu-2 NCs

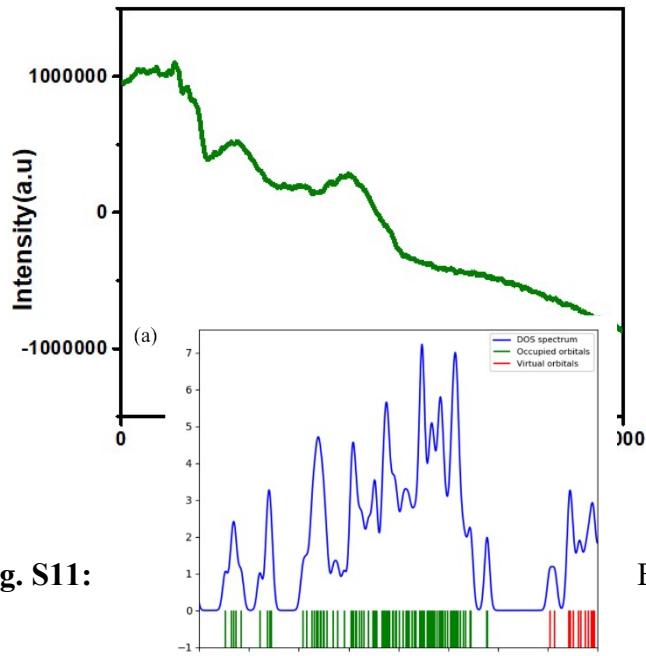


Fig. S11:
EPR spectrum of AuCu-2
NCs.

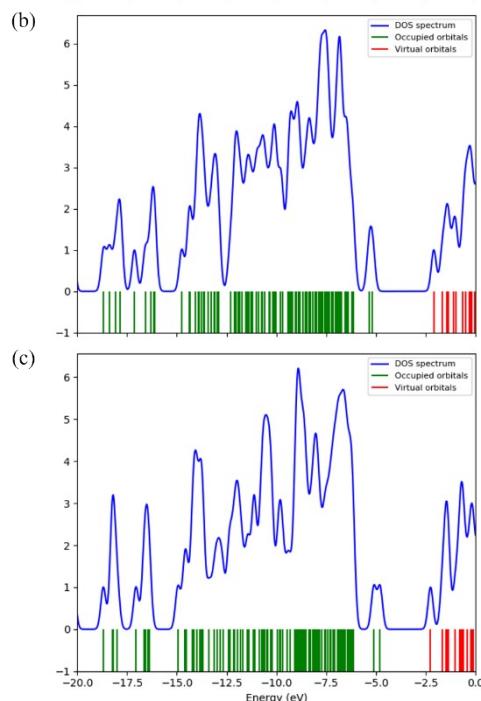


Fig. S12: DOS plot for (a) Au, (b) AuCu-1, and (c) AuCu-2 NCs

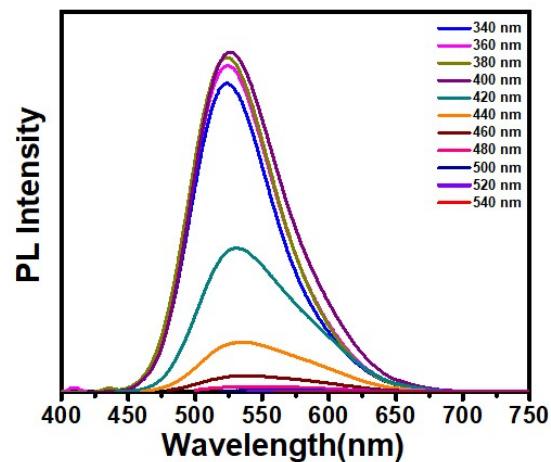


Fig. S13: Excitation-dependent PL of Au NCs.

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

Systems	Au 4f_{7/2} B.E (eV)	Au4f_{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

