

Supporting Information

Tailoring the Photoluminescence of AIE-Type Gold Nanoclusters via Biomineralization-Inspired Polymorphism

Sukhendu Mahata^{a,b}, Satya Ranjan Sahoo^{a,b}, Arun Mukhopadhyay^{a,b}, Komal Kumari^c, Surajit Rakshit^c and Nirmal Goswami^{a,b*}

^aMaterials Chemistry Department, CSIR-Institute of Minerals and Materials Technology, Bhubaneswar 751013, Odisha, India.

^bAcademy of Scientific and Innovative Research (AcSIR), Ghaziabad 201002, Uttar Pradesh, India.

^cDepartment of Chemistry, Institute of Science, Banaras Hindu University, Varanasi 221005, Uttar Pradesh, India.

Corresponding Author's Email: ngoswami@immt.res.in

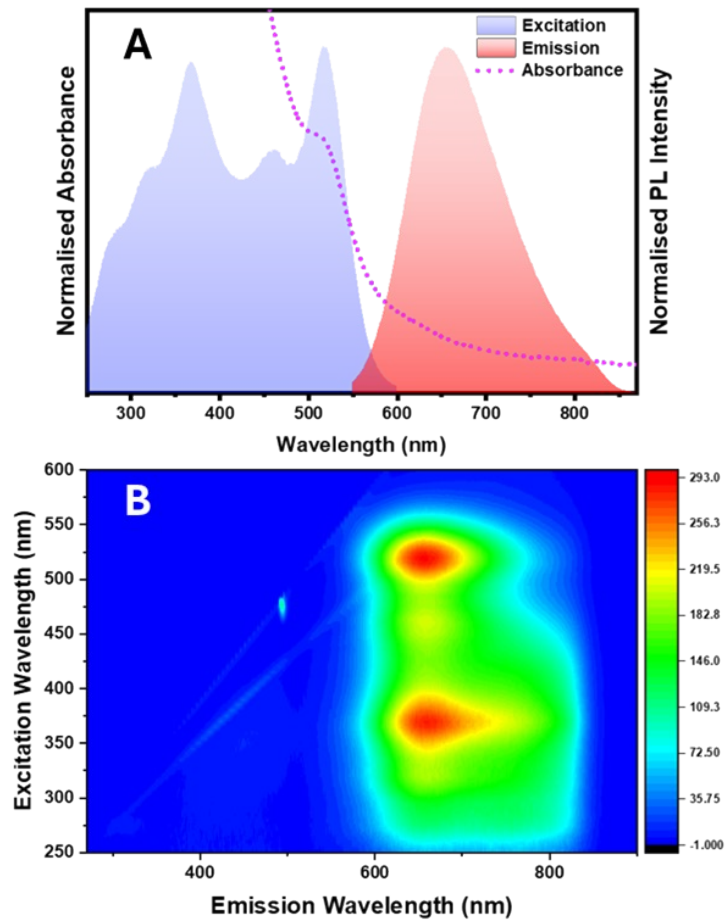


Fig. S1. (A) Excitation, Emission and Absorbance spectrum of $\text{Au}_{22}\text{SG}_{18}$. (B) 2D Excitation Emission spectra of $\text{Au}_{22}\text{SG}_{18}$. ($\lambda_{\text{ex}} = 520 \text{ nm}$)

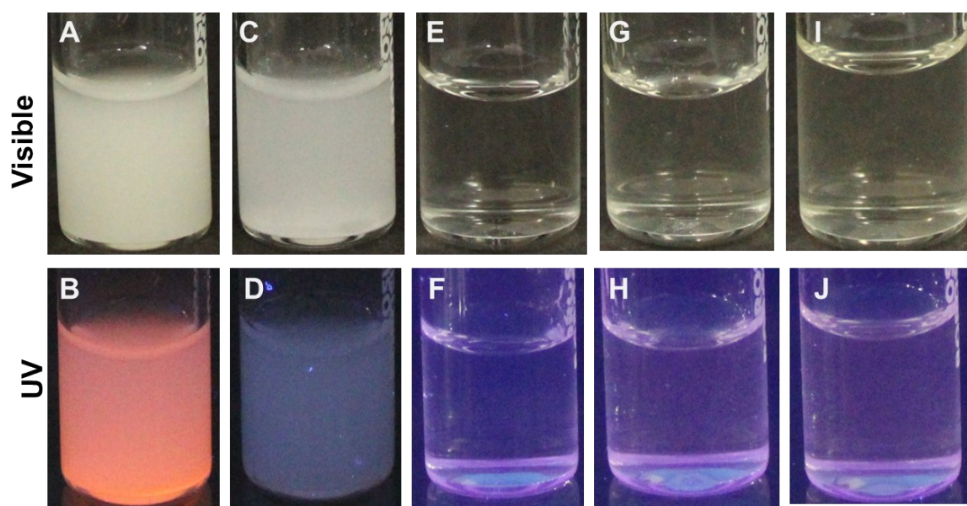


Fig. S2. Photographic images of $\text{Au}_{22}\text{SG}_{18}$ @ CaCO_3 -Cube (A-B), CaCO_3 - Cube (C-D), CaCl_2 in EG/water (E-F), $\text{Au}_{22}\text{SG}_{18}/\text{CaCl}_2$ in EG/water (G-H), $\text{Au}_{22}\text{SG}_{18}$ in EG/water (I-J) under UV and visible light.

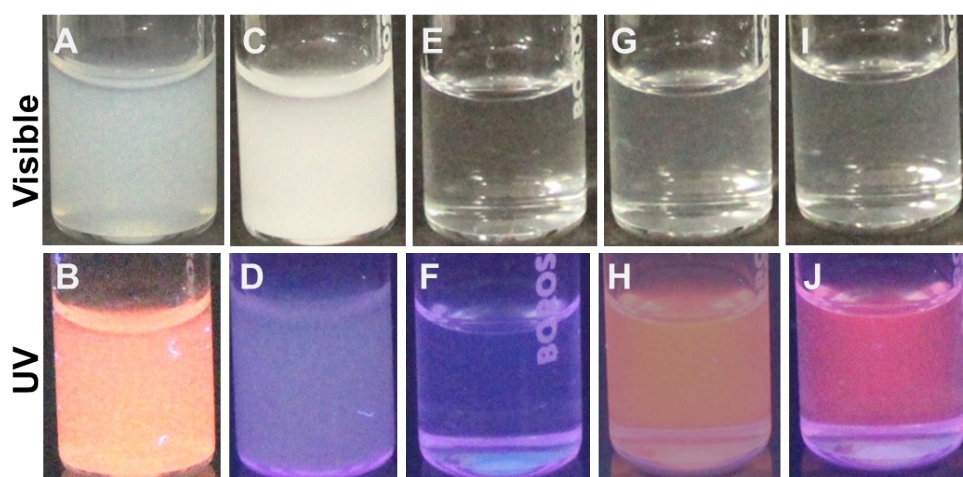


Fig. S3. Photographic images of Au₂₂SG₁₈ @CaCO₃-Cube/Sphere(A-B), CaCO₃-Cube/Sphere(C-D), CaCl₂ in water-ethanol (E-F), Au₂₂SG₁₈/ CaCl₂ in water-ethanol (G-H), Au₂₂SG₁₈ in water-ethanol(I-J)

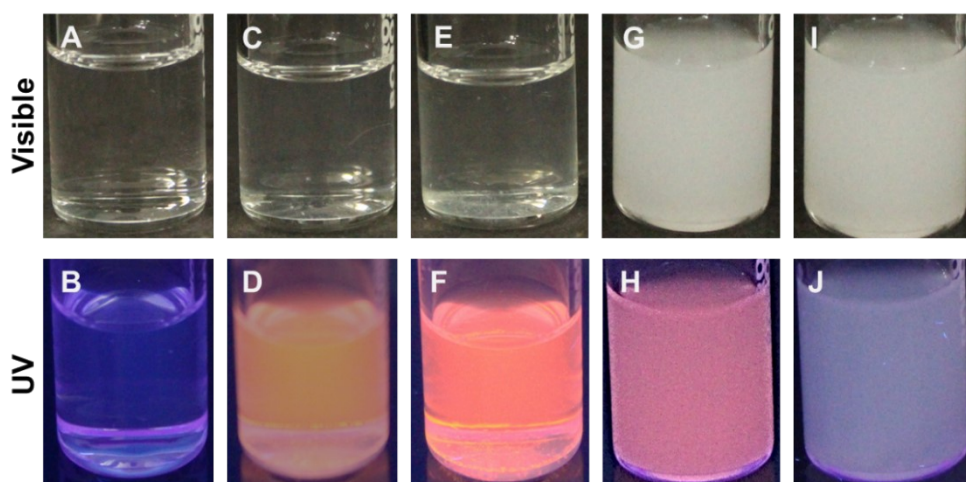


Fig. S4. Photographic images of CaCl₂ in ethanol/water (A-B), Au₂₂SG₁₈/CaCl₂ in ethanol/water(C-D), Au₂₂SG₁₈ in ethanol/water (E-F), Au₂₂SG₁₈ @CaCO₃ -sphere (G-H), CaCO₃ -Sphere(I-J)

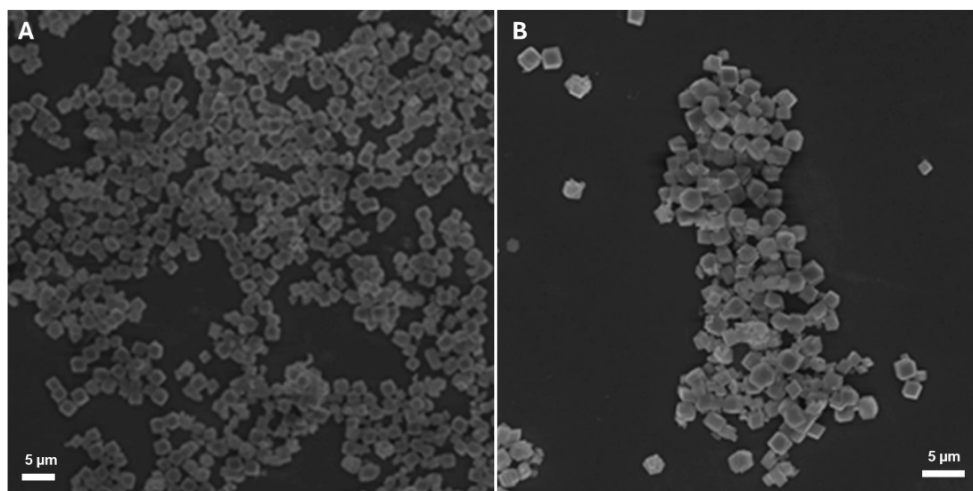


Fig. S5. FESEM images of CaCO₃-Cube-control

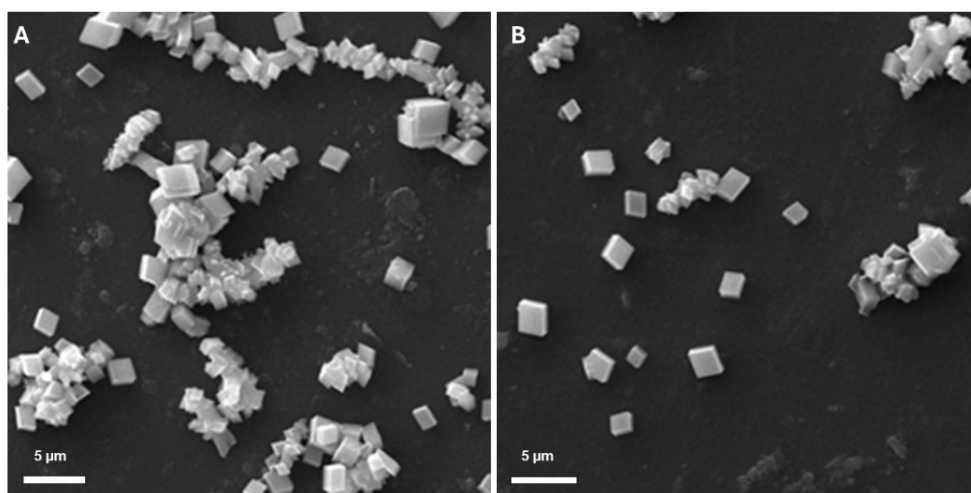


Fig. S6. FESEM image of CaCO₃-Cube/Sphere-control

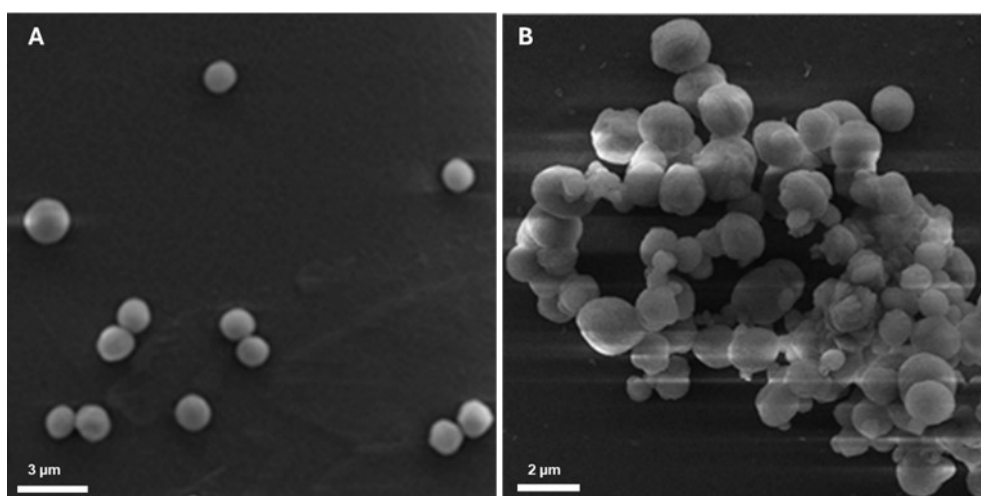


Fig. S7. FESEM images of CaCO₃-Sphere-Control

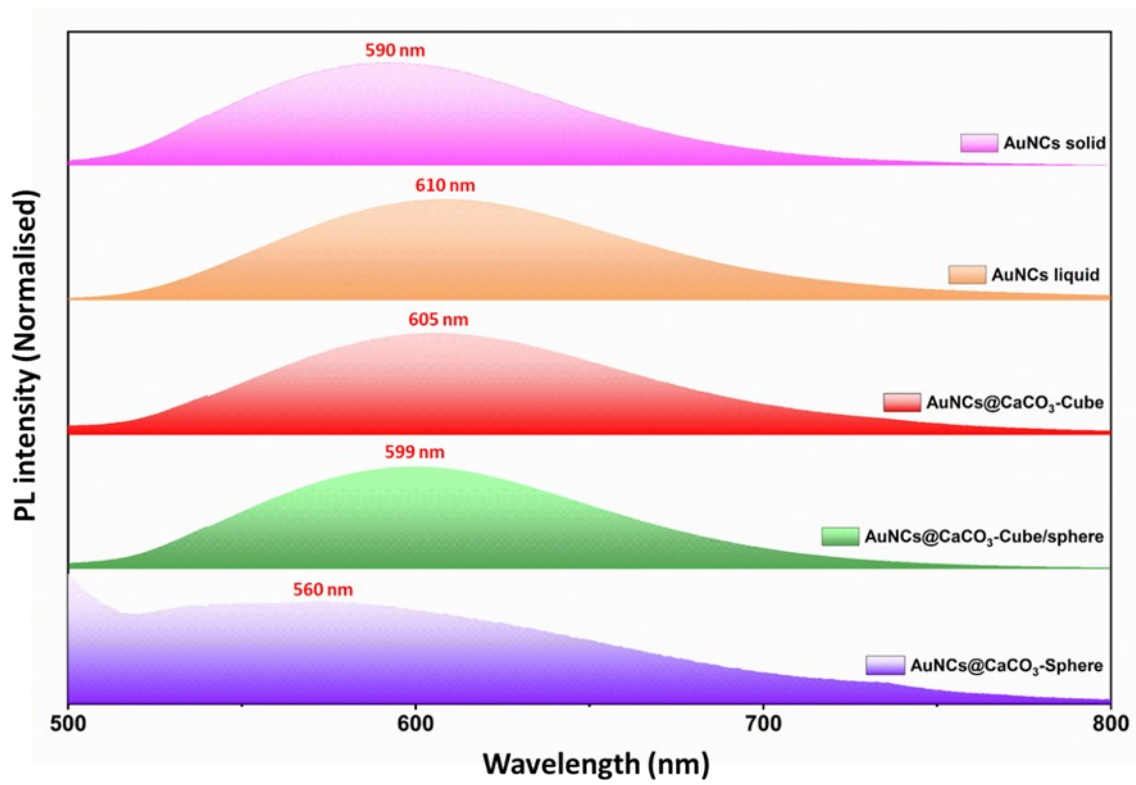


Fig. S8. PL intensity of AuNCs@CaCO₃-composites (excitation wavelength = 375 nm).

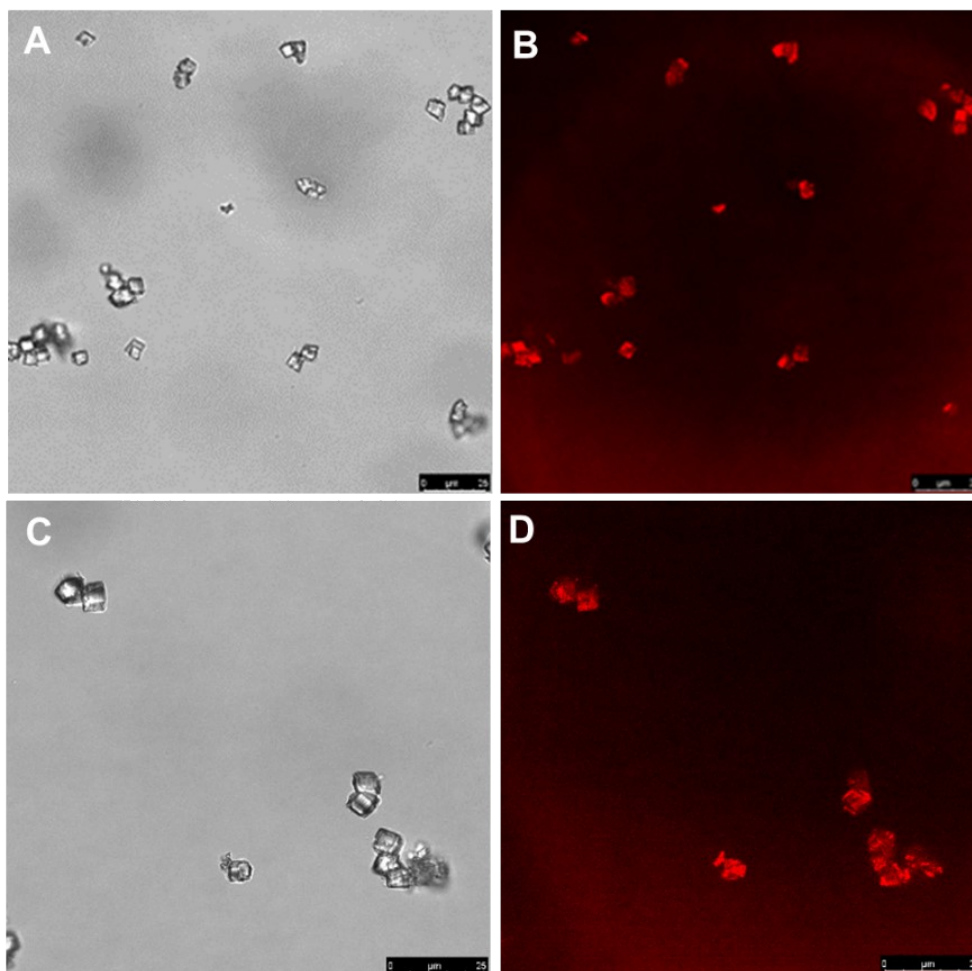


Fig. S9. Confocal microscopic images of $\text{Au}_{22}\text{SG}_{18}@\text{CaCO}_3\text{-Cube}$

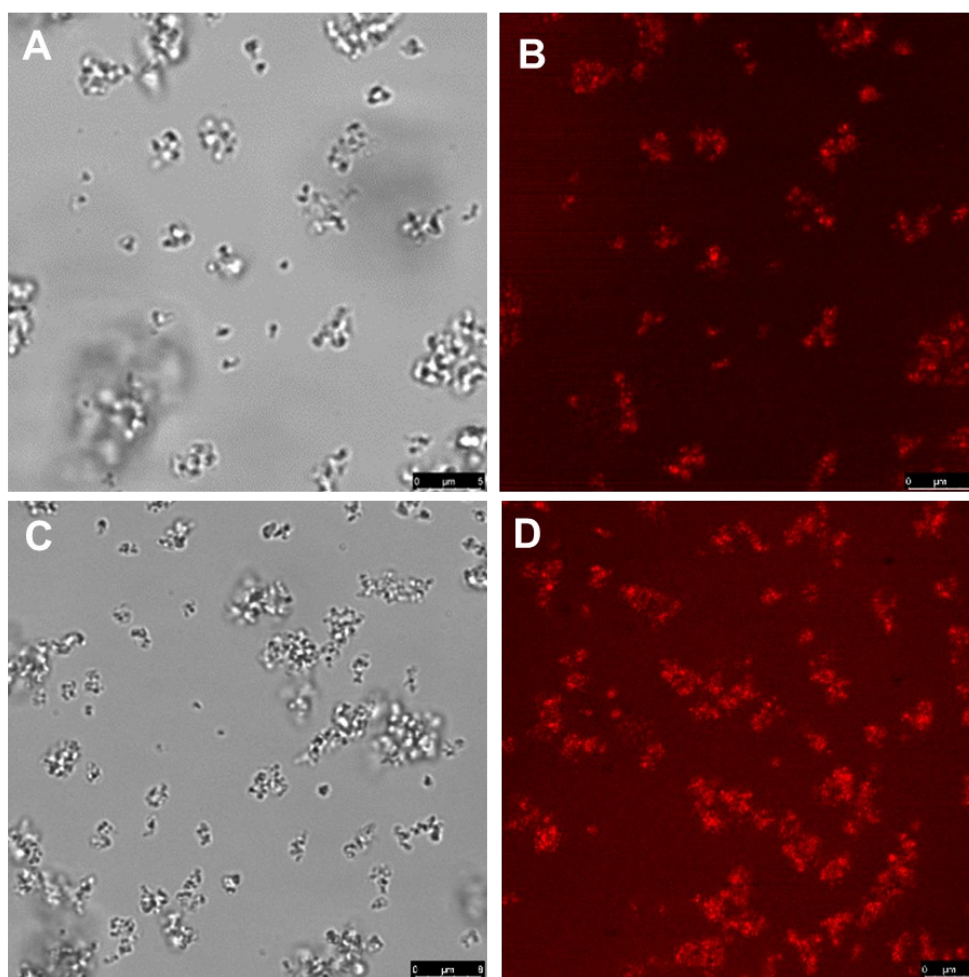


Fig. S10. Confocal microscopic image of $\text{Au}_{22}\text{SG}_{18}@\text{CaCO}_3$ -Sphere

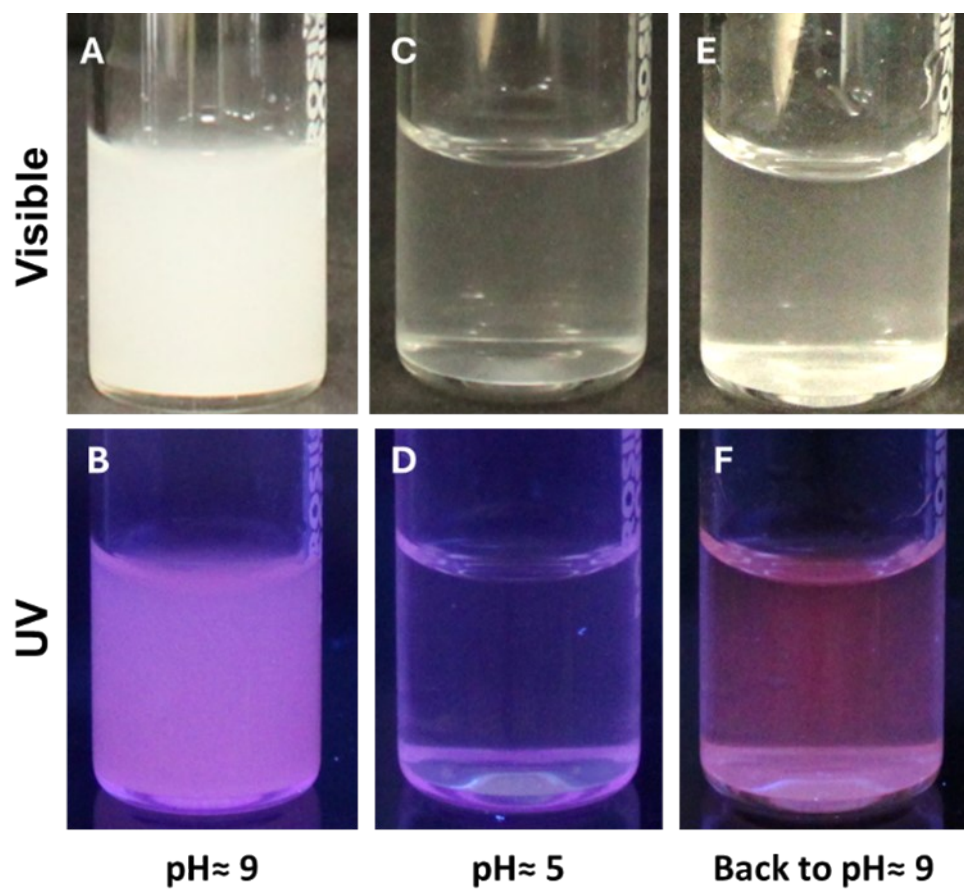


Fig. S11. Photographic images of $\text{Au}_{22}\text{SG}_{18} @\text{CaCO}_3$ -Cube at different pH under visible and UV light, at pH \approx 9 (A-B), pH \approx 5 (E-D), back to pH \approx 9 (E-F).

Table S1. Summary of lifetime values of as synthesized Au₂₂SG₁₈ NCs embedded CaCO₃ matrices in microsecond time scale. Excitation wavelength = 375 nm; emission wavelength = 660 nm.

Samples	A ₁	τ ₁ (ns)	A ₂	τ ₂ (ns)	A ₃	τ ₃ (ns)	τ _{avg} (ns)
Au ₂₂ SG ₁₈ @CaCO ₃ -Cube	1049.07	1477.57	4074.15	8988.54	0	0	7450.53
Au ₂₂ SG ₁₈ @CaCO ₃ -Cube/Sphere	2976.56	2580.48	2425.08	10433.34	0	0	6106.04
Au ₂₂ SG ₁₈ @CaCO ₃ -Sphere	3628.95	1963.96	1734.56	9179.09	0	0	4297.33
Au ₂₂ SG ₁₈	2734	209.5	1980	1038	548.4	3426	856.51

Table S2. Summary of lifetime values of as synthesized Au₂₂SG₁₈ NCs embedded CaCO₃ matrices in nanosecond time scale. Excitation wavelength = 375 nm; emission wavelength = 660 nm.

Samples	A ₁	τ ₁ (ns)	A ₂	τ ₂ (ns)	A ₁ +A ₂	A ₁ /(A ₁ +A ₂)	A ₂ /(A ₁ +A ₂)	τ _{avg} (ns)
Au ₂₂ SG ₁₈ @CaCO ₃ -Cube	0.010	76.714	0	0	0.01	1	0	76.714
Au ₂₂ SG ₁₈ @CaCO ₃ -Cube/Sphere	0.011	45.746	0	0	0.011	1	0	45.746
Au ₂₂ SG ₁₈ @CaCO ₃ -Sphere	0.026	1.233	0.009	35.7956	0.035	0.743	0.257	10.121
Au ₂₂ SG ₁₈ solid	0.005	25.387	0	0	0.005	1	0	25.387
Au ₂₂ SG ₁₈ liquid	0.035	1.150	0.016	38.565	0.051	0.686	0.314	12.887

Table S3: The atomic concentration of gold in each composite determined by ICP-OES.

Material	Amount of Au in 1 mg composite (mg)
Au ₂₂ SG ₁₈ @CaCO ₃ -Cube	1.591 × 10 ⁻²
Au ₂₂ SG ₁₈ @CaCO ₃ -Cube/Sphere	0.684 × 10 ⁻²
Au ₂₂ SG ₁₈ @CaCO ₃ -Sphere	0.796 × 10 ⁻²

