Supporting information

Hybrid-biotaxonomy-like machine learning enables an anticipated surface plasmon resonance of Au/Ag nanoparticles assembled on ZnO nanorods

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Section S1. The detailed processes to synthesize 5 species of noble metal NPs colloid

Synthesis of gold nanorods colloid: gold nanorods (AuNRs) were synthesized by a seed-mediated approach. Seed solution was first prepared by adding 0.6 mL 10 mM sodium borohydride into 10 mL aqueous solution containing 0.1 M CTAB and 5×10^{-4} M $HAuCl_4$. Then, the growth solution was prepared by mixing 5-7 mL 10^{-3} M $HAuCl_4$ (X_2), 5 mL 0.2 M CTAB, 250 μL $4x10^{-3}$ M $AgNO_3$, and 70 μL 0.0788 M ascorbic acid with a gentle stirring. Next, 12 μL seed solution was added to the growth solution and left still for 24 h to complete the rod growth. Before use, the AuNRs colloid was centrifugated at 10000 rpm for 40 min and then suspended in ethylene glycol.

Synthesis of Au seeds for ULANPs and S-Au-AgNPs: The Au seed solution was synthesized by the citrate-reduction method. Seed solution was prepared by adding 5 mL 38.8 mM sodium citrate into 50 mL 0.5 mM $HAuCl_4$ aqueous solution, which was magnetically stirred at 600 rpm at 100 °C until the solution became red.

Synthesis of urchin-like AuNPs colloid: The 240 μL Au seed solution was firstly added into 120 mL 10^{-4} M $HAuCl_4$ stirred at 600 rpm at room temperature for 5 min to form an aqueous solution. Then, 5 mL 38.8 mM sodium citrate was added to the above solution to react for 5 min. Subsequently, 20 mL 30 mM hydroquinone was added to the solution and stirred for 30 min.

Synthesis of S-Au-AgNPs colloid (4^{th} layer): The preparation of S-Au-AgNPs colloid was similar to ULANPs colloid. For 4^{th} layer S-Au-AgNPs(575), 500 μL Au seed solution and 60 mL 0.1 mM $AgNO_3$ were added into 100 mL 10^{-4} M $HAuCl_4$, which was stirred at 600 rpm at room temperature for 5 min to form an aqueous solution. Then, after completely mixing, sodium citrate (38.8 mM, 200 μL) and hydroquinone aqueous solution (30 mM, 30 mL) was added to the solution one by one, and the solution was stirred for 12 h.

Synthesis of S-Au-AgNPs colloid (5^{th} layer): For S-Au-AgNPs(5^{th} layer), all the preparation process was analog to the 4^{th} layer process. 50 μL Au seed solution and 3-6 mL 0.1 mM $AgNO_3$ (X_5) were added to 10 mL 10^{-4} M $HAuCl_4$, which was stirred at 600 rpm at room temperature for 5 min to form an aqueous solution. Then, after completely mixing, sodium citrate (38.8 mM, 20 μL) and hydroquinone aqueous solution (30 mM, 3 mL) was added to the solution one by one, and the solution was stirred for 12 h.

Synthesis of S-AgNPs colloid: 0.5 mM polyvinylpyrrolidone (PVP) powder was first dissolved in 20 mL ethylene glycol. Then, $AgNO_3$ powder was added to the PVP solution to form 0.025-0.050 M $AgNO_3$ (X_6) solution by magnetically stirring until the color changed to yellow. Subsequently, 0.05 M sodium borohydride was added to the above solution and stirred for 30 min.

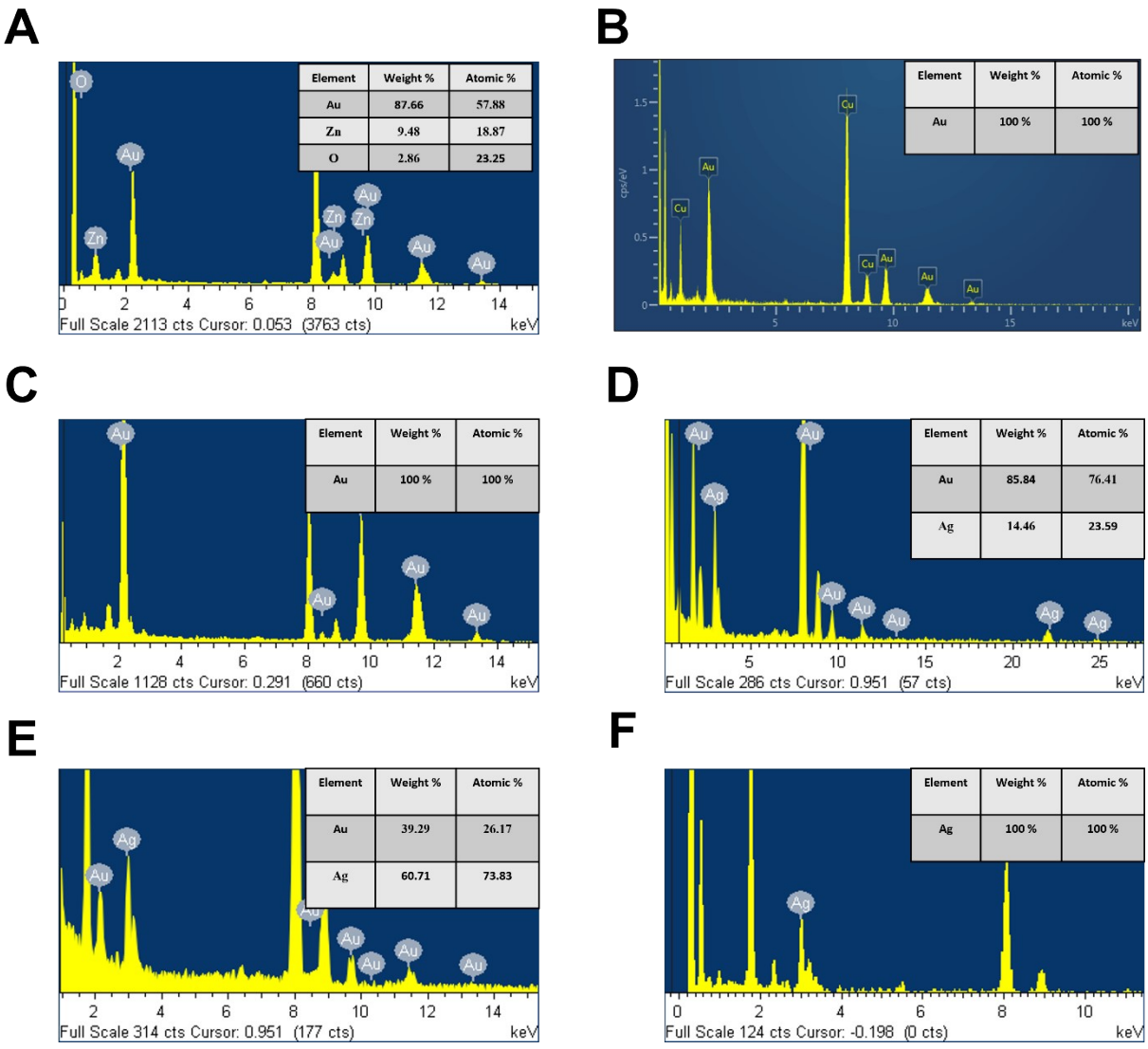

Fig. S1. Energy dispersive X-ray (EDX) spectrum of six species of NMNPs through transmission electron microscopy (TEM) analysis. (A) S-Au/ZnONRs, (B) AuNRs, (C) ULANPs, (D) S-Au-AgNPs (molar ratio Au/Ag=3), (E) S-Au-AgNPs (molar ratio Au/Ag=1/3), and (F) S-AgNPs.

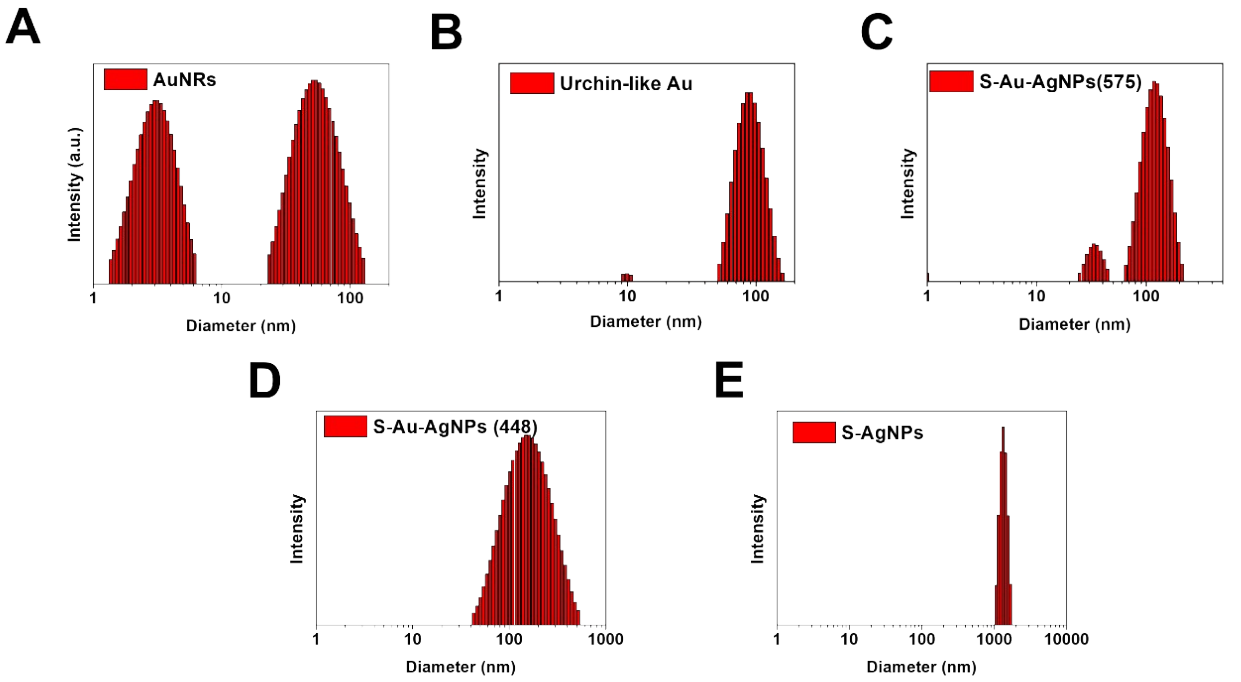

Fig. S2. Size distribution of five species of NMNPs suspended in the colloid. (A) AuNRs, (B) ULANPs, (C) S-Au-AgNPs (molar ratio Au/Ag=3), (D) S-Au-AgNPs (molar ratio Au/Ag=1/3), and (E) S-AgNPs.

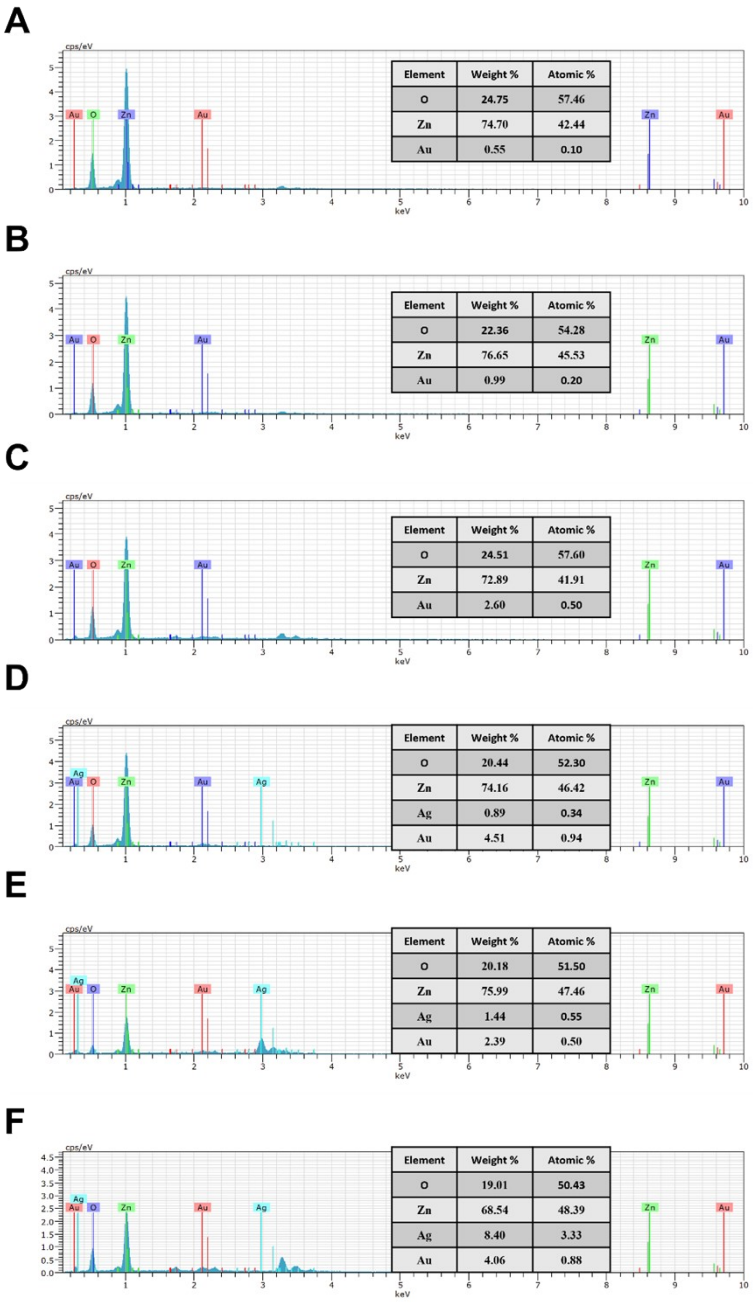

Fig. S3. EDX spectrum of six-layer NMNPs on ZnONRs through scanning electron microscopy (SEM) analysis. (A) S-Au/ZnONRs, (B) AuNRs/S-Au/ZnONRs, (C) ULA/AuNRs/S-Au/ZnONRs, (D) S-Au-Ag(575)/ULA/AuNRs/S-Au/ZnONRs, (E) S-Au-Ag/S-Au-Ag(575)/ULA/AuNRs/S-Au/ZnONRs, and (F) S-Ag/S-Au-Ag/S-Au-Ag(575)/ULA/AuNRs/S-Au/ZnONRs.

Table S1. Measured cumulant diameter and zeta potential of 5 species of NMNPs suspended in the colloid.

	Measured cumulant diameter (nm)	Measured zeta potential (mV)
AuNRs	**35.6**	**39.62**
ULANPs	**75.4**	**-42.53**
S-Au-AgNPs (575)	**94.4**	**-41.74**
S-Au-AgNPs (448)	**132.7**	**21.36**
S-AgNPs	**1532.2**	**-2.37**