SUPPORTING INFORMATION

Mono and bimetallic nanoparticles for catalytic degradation of hazardous organic dyes and anti-bacterial applications

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**Figure S1.** (a) Schematic representation of the FDTD simulations. Synthesized NPs in the water medium background are being illuminated by a plane-wave source whose propagation vector is in the negative z-direction while the electric (E) field is oscillating along the x-axis. Here, d-diameter, P-periodicity E-electric field vector, k-propagation vector (b) Real simulation environment with applied symmetry boundary conditions (BCs). Here, NP-nanoparticle, T-transmittance monitor, R-reflectance monitor

**Figure S2.** EDAX spectra of (a) AuAg and (b) CuAg BMPs, Inset: Elemental composition of Au and Ag in AuAg BMNPs.
The formation of AuAg and CuAg BMNPs is confirmed by EDAX spectra (Figure S2(a and b) and Figure S3(a and b)). The elemental composition of monometallic counterparts is illustrated in the inset table.
Figure S4. Simulated and measured absorbance spectra comparison for (a) Au (b) Ag (c) Cu (d) AuAg and (e) CuAg NPs indicating their $\lambda_{\text{max}}$. The simulation parameters are taken as summarized in Table S1 based on the structural characterization obtained in Figure 2 of the main manuscript

**Effect of pH on morphology and absorption spectra**

The synthesis of metal nanomaterials is pH sensitive. Here, HCl and NaOH are used to vary the pH. At lower pH, as the H$^+$ increases, the number of electrons available for reduction reaction is less and hence reaction may not take place. Hence SPR peak may not be observed in optical spectra. On the other hand, the poor balance between nucleation and growth results in bigger and irregular-shaped particles due to agglomeration, causing the broadening and redshift of the SPR peak. In general, for particles $>15$ nm as particle size increases, so does the spectral width and redshift of the SPR peak position due to increased scattering at higher wavelengths and vice versa for smaller particles.$^1$ Further, the lack of electrons results in a higher agglomeration tendency due to lower electrostatic repulsion. As the pH increases, the rate of reduction is increased and thus a balance between nucleation and growth is achieved due to the presence of an excess of electrons (OH$^-$ ions). As a result, the basic condition is the favorable environment for the synthesis of metal nanoparticles. In the present work, except for the synthesis of Au and AuAg NPs, the latter statement is true. On the other hand, the repulsive electrostatic interaction reduces the possibility of agglomeration. Hence monodispersed small nanoparticles are formed resulting in intense sharp peak$^{1,2}$. On further increasing the pH, the rapid nucleation compared to slow growth results in larger, non-uniform particles thus causing broadening of the SPR peak.$^{2,4}$
The contradictory behavior of Au and Ag nanoparticles i.e., narrow SPR peaks are observed, which indicate the formation of small, monodispersed particles at acidic pH. This can be explained on the basis of the reaction mechanism of reducing agent, trisodium citrate used in both the cases. During the reduction reaction of Au salt, citrate gets oxidized by yielding dicarboxy acetone. Meanwhile, by utilizing the electrons from the citrate oxidation reaction, Au(III) salt gets reduced into Au(I) salt. At lower pH, as the H⁺, the citrate oxidation rate may increase and hence the increased number of electrons results in the higher rate of reduction achieving a balance between nucleation and growth. However, on further decreasing the pH, large number of H⁺ ions limit the availability of electrons for the reduction.³

In the current study, during the synthesis of Au NPs, the concentration of trisodium citrate NPs is relatively high, yielding a greater number of electrons for the reduction reaction. Hence, small, monodispersed Au particles are formed at pH 2, which is evident from the sharp and intense SPR peak. However, in the case of AuAg BMPs, pH 4 is the optimum pH. At pH 2, a slight increase in spectral width, diminished and redshift of SPR peak is noticed. This may be due to the decreased reduction rate caused by the lack of electrons due to the low concentration of trisodium citrate compared to Au seed solution and the concentration of Ag salt solution resulting in slightly larger particles.⁴

We sincerely apologize for our inability in obtaining slots for FESEM characterization. We approached a few of the central facilities for FESEM, unfortunately, we are not able to get the slots for analysis at this moment due to the nonworking condition of the instruments. However, we were successful in obtaining slots for TEM analysis for BMPs, which is detailed above.
Figure S5. Electric field intensity (E) profiles of (a) Au (b) Ag (c) Cu (d) AuAg and (e) CuAg NPs at their $\lambda_{\text{max}}$. 

$|E|^2$ (V/m)$^2$
Figure S6. Power absorption profiles of (a) Au (b) Ag (c) Cu (d) AuAg and (e) CuAg NPs at their $\lambda_{\text{max}}$. 

$P_{\text{abs}}$ (W)
Figure S7. Current density profiles of (a) Au (b) Ag (c) Cu (d) AuAg and (e) CuAg NPs at their $\lambda_{\text{max}}$.

Figure S8. Deconvolution of XRD of CuAg BMPs in the range 2$\theta$ from 40° to 54° using Fityk software.
Figure S9. Absorption spectra of Rhodamine B in the presence of NaBH₄ and (a) Au (b) Ag (c) Cu (d) AuAg (e) CuAg BMPs (f) Absorption spectra of Rhodamine B in the presence of NaBH₄ alone. Optical image of Rhodamine B dye before and after catalytic degradation (Inset)
Figure S10. Absorption spectra of indigo carmine dye in the presence of NaBH₄ and (a) Au (b) Ag (c) Cu (d) AuAg (e) CuAg BMPs (f) Absorption spectra of indigo carmine in the presence of NaBH₄ alone. Optical image of Indigo Carmine dye before and after catalytic degradation (Inset).
Figure S11. In \(\frac{A_0}{A_t}\) Vs time plot for the degradation of 4-nitrophenol dye in the presence of NaBH₄ and (a) Au (b) Ag (c) Cu (d) AuAg (e) CuAg NPs (f) without catalyst.
Rhodamine B dye shows the main characteristic absorption band at wavelength 554 nm. This band is due to the color of the dye and the intensity of this band is used for monitoring the decolorization of the dye. It is evident from the Figure. S9 (a-e) that Au, Ag, Cu, AuAg, and CuAg NPs degraded the rhodamine B dye, and the rate constants of the catalytic reactions are measured to be 0.0058 sec$^{-1}$, 0.0005 sec$^{-1}$, 0.0032 sec$^{-1}$, 0.0066 sec$^{-1}$ and 0.0317 sec$^{-1}$ respectively (Figure. S12(a-e)). The corresponding percentages of degradation of dye using Au, Ag, Cu, AuAg, and CuAg as catalysts are found to be 87.25%, 53.64%, 92.44%, 91.20% and 97% in 6 minutes, 21 minutes, 14 minutes, 6 minutes and 3 minutes respectively. Whereas only 4.64% degradation of rhodamine B for 20 minutes is observed without metal catalysts and rate constant is measured to be 0.00003 sec$^{-1}$ (Figure. S9f and S12f).
The synthesized mono and bimetallic nanoparticles showed high catalytic efficiency for the degradation of indigo carmine dye. The progress of the reaction is studied by observing the decrease in intensity of the characteristic band of indigo carmine dye at 611 nm (Figure S10(a-e)) which is responsible for the color of the dye. From Figure S13(a-e), rate constants of the catalytic reactions in the presence of Au, Ag, Cu, AuAg and CuAg NPs are calculated to be 0.0147 sec$^{-1}$, 0.0157, 0.0102 sec$^{-1}$, 0.0055 sec$^{-1}$, and 0.0212 sec$^{-1}$, respectively. In addition, the dye exhibited 97.08%, 94.89, 84.66%, 88.59% and 72.04% of degradation in 4 minutes, 3 minutes, 3 minutes, 6 minutes and 1 minute individually (Figure 10(a-e)). From Figure S10f and S13f, it can be observed that, in the absence of metal catalysts, the percentage degradation is 51.38% in 20 minutes and the corresponding rate constant is measured to be 0.0005 sec$^{-1}$. 

Figure S13. ln ($A_0$/$A_t$) Vs time plot for the degradation of indigo carmine dye in the presence of NaBH$_4$ and (a) Au (b) Ag (c) Cu (d) AuAg (e) CuAg NPs (f) NaBH$_4$ alone.
Figure S14. Mueller-Hinton Agar diffusion method for evaluating antibacterial activity of Au, Ag, and Cu NPs
(a) MRSA (b) Shigella flexneri (c) Salmonella ser. Typhimurium (d) Klebsiella pneumoniae (e) Acinetobacter baumannii (f) Enterococcus faecium.
Figure S15. Inactivity of Au, Ag, Cu, AuAg and CuAg NPs towards (a) *Escherichia coli* (b) *Aeromonas hydrophilia* and (c) *Vibrio cholerae*

The inactivity of Ag NPs towards certain bacteria like *Vibrio cholerae*, *Escherichia coli* and *Aeromonas hydrophila* might be due to the reason that negatively charged trisodium citrate capping agent inhibits the physical interaction of NPs with cell wall due to electrostatic repulsion.
Table S1: FDTD Simulation parameters correlating the experimental and simulation $\lambda_{\text{max}}$

| Nano Particle | Composition Ratio (%) | Diameter (d) (nm) | Periodicity (P) (nm) | $\lambda_{\text{max}}$ (nm) |
|---------------|-----------------------|-------------------|----------------------|-----------------------------|
|               |                       | x | y | z | x | y | Measured | Simulated |
| Au            | 100                   | 15| 20 | 525 | 542 |
| Ag            | 100                   | 25| 40 | 425 | 411 |
| Cu            | 100                   | 65| 95 | 583 | 556 |
| AuAg          | 90:10                 | 30| 40 | 417 | 430 |
| CuAg          | 70:30                 | 50| 45 | 40 | 395 | 412 |
Table S2. Inhibition zone diameter of Ag samples for various bacteria

| Name of the bacteria                   | Diameter of the inhibition zone for Ag sample (mm) |
|----------------------------------------|---------------------------------------------------|
| *Pseudomonas aeruginosa*               | 12                                                |
| *Shigella flexneri*                   | 11                                                |
| *Enterococcus faecium*                 | 11                                                |
| *Acinetobacter baumannii*              | 10                                                |
| *Staphylococcus aureus*                | 10                                                |
| *Salmonella ser. Typhimurium*          | 8                                                 |
| *Klebsiella pneumoniae*                | 7                                                 |
| *Vibrio cholerae*                     | NIL                                               |
| *Escherichia coli*                    | NIL                                               |
| *Aeromonas hydrophila*                 | NIL                                               |

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