MXene@AgAu@PDA nanoplatform loaded with AgAu nanocages for enhancing catalytic activity and antibacterial performance

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Fig. S1. Digital image of MXene aqueous solution with a typical Tyndall effect.

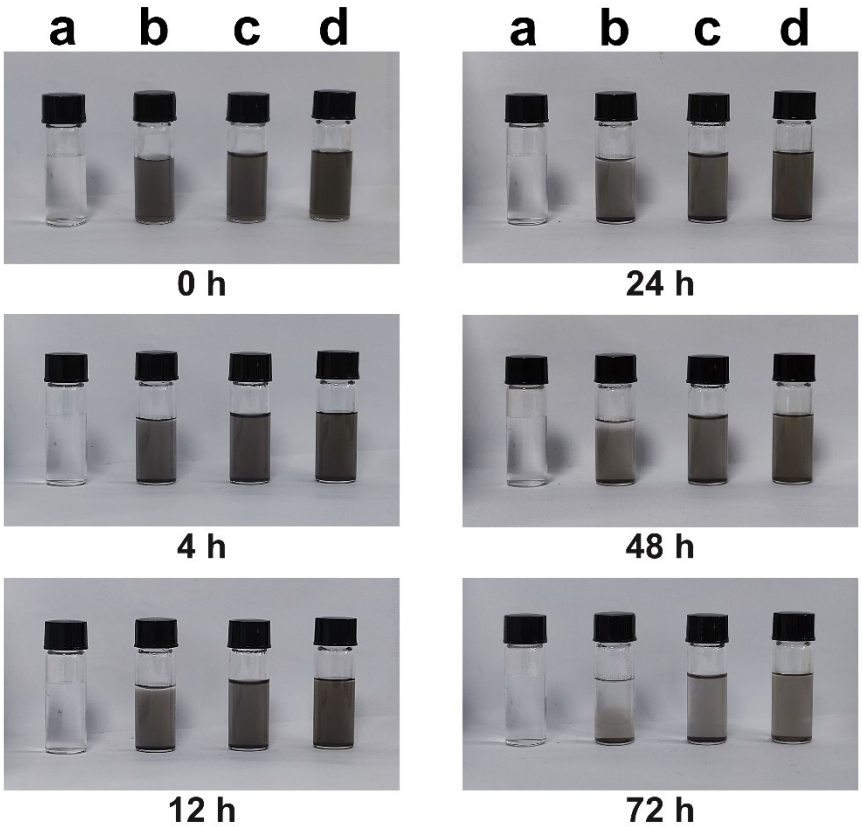

Fig. S2. The stability of 40 μg·mL^{-1} MXene@AgAu@PDA nanosheets in water, ethanol, and N, N-Dimethylformamide (DMF) three commonly used solvents over time. (a: H_2O; b: H_2O + 40 μg·mL^{-1} MXene@AgAu@PDA; c: ethanol + 40 μg·mL^{-1} MXene@AgAu@PDA; d: DMF + 40 μg·mL^{-1} MXene@AgAu@PDA)

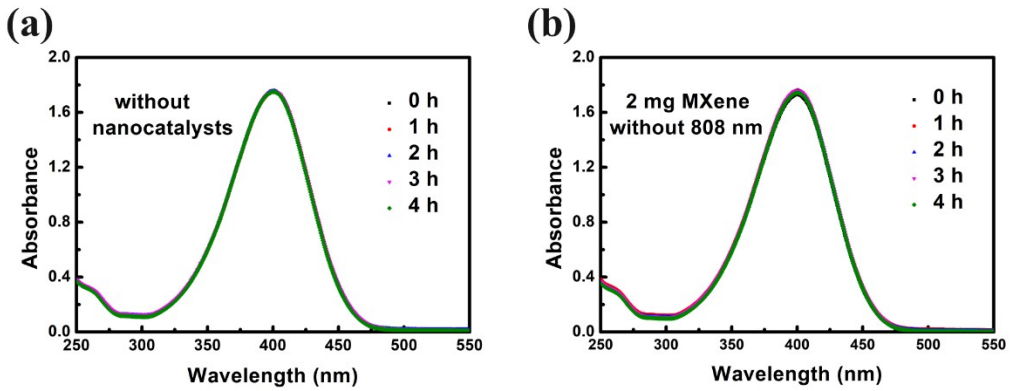

Fig. S3. Time-dependent absorption spectra for the catalytic reduction of 4-nitrophenol by (a) none and (b) 2 mg MXene under dark conditions.

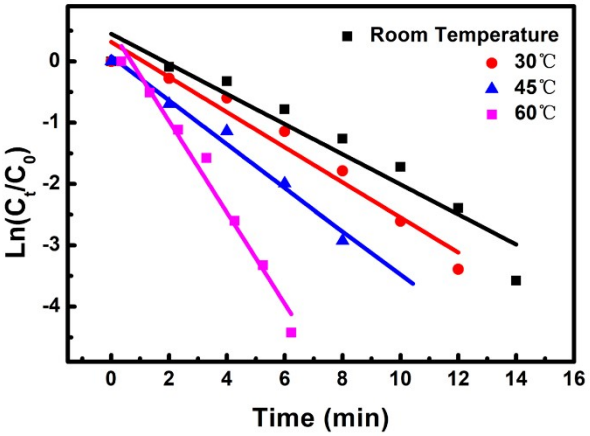

Fig. S4. The linear relationship between the reaction time and $Ln(C_t/C_0)$ of MXene@AgAu@PDA nanocatalysts with different oil bath temperatures. The results showed that the catalytic activity increased with the increase of temperature.

Computational Details

The density functional theory (DFT) calculation were carried out using Vienna Ab initio Simulation Package (VASP). The exchange–correlation energy functional was described by Perdew-Burke-Ernzerhof generalized gradient approximation (GGA-PBE) and the projector augmented wave (PAW) pseudopotentials was used to describe the core electrons interaction. The KPOINTS mesh density was 4×3×1 using Gamma center scheme, and the plane wave energy cutoff was set to 350 eV. The vacuum region was set to 10 Å. The energy convergence threshold was set to 10^{-6} eV and the force

threshold was set to 0.01 eV/Å during structure optimization.

The charge density difference was calculated by the formula,

$$\Delta\rho = \rho\left(AgAu@Ti_3C_2O_2\right) - \rho(AgAu) - \rho(Ti_3C_2O_2)$$

Where the ρ(AgAu@$Ti_3C_2O_2$), ρ(AgAu), ρ($Ti_3C_2O_2$) is the charge density of AgAu@$Ti_3C_2O_2$, AgAu and $Ti_3C_2O_2$ respectively.