Electronic Supplementary Information (ESI)

Environmental friendly InP quantum dots as visible-light catalyst for water treatment

Synthesis of oleylamine-capped InP QDs. InCl₃ (99.5 mg, 0.45 mmol, 1 eq.), ZnCl₂ (307 mg, 2.25 mmol, 5 eq.) and oleylamine (5 mL) were added to a 50 mL three-necked roundbottomed flask in an argon-filled glovebox. The flask was equipped with a reflux condenser and connected to a Schlenk line. A temperature probe was inserted through one of the necks and the last one was equipped with a septum to allow the addition of reagents. The mixture was heated at 120°C under vacuum (0.20 mbar) to dissolve metal salts and remove oxygen and water traces. The flask was then filled with argon and the temperature was set to 180°C before the injection of trisdiethylaminophosphine (P(DEA)₃) (0.49 mL, 1.80 mmol, 4 eq.). After 20 min, the mixture was cooled to room temperature, by immersing the flask in an ice-water bath. 20 mL of chloroform was added in the reaction mixture. A first centrifugation was performed at 7000 rpm during 7 min to remove the unreacted salts. Then, purification was completed with 2 cycles of centrifugation with an absolute ethanol-chloroform (v/v 4:1) mixture. The QDs were suspended in 10 mL of chloroform in a 10 mL screw-cap vial.

Ligand exchange with $(NH_4)_2S$. As-synthesized QD suspension (1.2 mL), chloroform (5 mL), formamide (1 mL) and a solution of $(NH_4)_2S$ (20 wt. % in water, 20 µL, 0.059 mmol) were added to a 25 mL round-bottomed flask. The solution was stirred until the QDs transitioned from the chloroform phase to the formamide one. The mixture was poured in a separatory funnel to remove the organic phase and the round-bottomed flask was washed with excess water. The aqueous phase was purified by 2 cycles of 1/3 (v/v) H₂O/acetone washing

resulting in precipitation of the QDs and centrifugation at 11400 rpm during 15 min. The mass concentration was determined by evaporating the solvent from an aliquot of 0.2 mL with a rotary evaporator and weighing the solid residue in the round-bottom flask. Then the solution was diluted in water to obtain a solution of 0.2 g.L^{-1} .

Characterizations of InP QDs concentration. The absorption of a photon will generate electron-hole pair which allows to determine the gap band following the equation (1):

$$\lambda = \frac{h.c}{E^{gap}} \tag{1}$$

with λ the wavelength at the excitonic peak.

The concentration of InP units, (InP)_i in the water solution and the concentration of nanocrystals (Nx) have been determined using the equation (2) and (3), based on previous studies (*Nat Commun 9*, 4009 (2018); *Chem. Mater.* 2015, 27, 13, 4893-4898; *Chem. Mater.* 2020, 32, 10, 4358-4368)

$$[InP_{i}] = A \frac{\ln(10) 1}{\mu_{i,th} l V_{M}}$$
⁽²⁾

$$[Nx] = \frac{[InP_i]}{N} \tag{3}$$

With A the absorbance at 413 nm, 1 the optical path length (1 cm), V_M the molecular volume of InP (3.0 × 10⁻⁵ m³.mol⁻¹), $\mu_{i,th}$ the intrinsic absorption coefficient (m⁻¹)and N the number of InP units in the crystal, N is given by equation (4):

$$N = \frac{L^3}{a_0^3 6\sqrt{2}}\tag{4}$$

Where, L is the edge length determined either by STEM or by calculation through the UV-Vis spectrum, and a_0 is the lattice constant of InP (0.5869 nm).



Figure S1 Size histogram corresponding to the InP QDs before ligand exchange.