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Supporting Information

Templating synthesis of dual-functional porous MoS₂ nanoparticles with photothermal conversion and catalytic properties

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Fig. S1 TEM images of (a) PS38.5k-*b*-P2VP23k and (b) PS48.5k-*b*-P2VP16.5k particles before swelling. The polymer particles were stained by I2 vapor for 20 min. The dark contrast shows the distribution of P2VP domains. SEM image of (c) PS38.5k-*b*-P2VP23k and (d) PS48.5k-*b*-P2VP16.5k particles after swelling at 50 °C. TEM images of the PS48.5k-*b*-P2VP16.5k particles swelling at (e) 30 and (f) 90 °C.



Fig. S2 TEM images of (a) MoS_2 PLNPs and (b) MoS_2 HNPs. The histograms of particle size distribution of the MoS_2 PNPs prepared at the precursor concentration of (c) 1, (d) 1.5 and (e) 3 mg/mL.



Fig. S3 XRD patterns of various MoS₂ PNPs.



Fig. S4 TGA curves of (a) various MoS_2 particles and (b) the chemical variation of the MoS_2 -1.5 PLNPs particles during calcination.

Taking MoS₂-1.5 PLNPs for example, the components change during calcination is as below:

$$3O_2(g) + MoS_2(s) \rightarrow MoO_3(s) + SO_3(g)$$
$$O_2(g) + C(s) \rightarrow CO_2(g)$$

Here we assume the initial amount of carbon and MoS_2 is *x* and *y*, respectively. The molar masses of MoS_2 and MoO_3 are 160.1 g/mol and 143.9 g/mol, respectively. Then the calculation equations of the mass equilibrium before and after calculation is below:

$$x + y = 100\%$$

$$\frac{143.9}{160.1} \times y = 55\%$$

Therefore, the amount of carbon and MoS_2 is calculated to be 38.9 % and 61.1 %. The results of various MoS_2 PNPs are summarized in **Table S1**.



Fig. S5 Isothermal N₂ adsorption and desorption of various MoS₂ particles. The insets are the corresponding curves of pore size distribution.



Fig. S6 Temperature change vs. time of MoS₂ particles with various morphologies when the laser on and off.



Fig. S7 TEM image of the MoS_2 -1.5 PNPs after 5 photothermal test cycles.



Fig. S8 Temperature change of water and various MoS_2 PNPs at 0.1 mg/ml under NIR irradiation at 3 W/cm².



Fig. S9 Photos of MoS₂ dispersions after storing for (a) 0 h, (b) 1.5 h and (c) 3h.



Fig. S10 TEM image of the MoS₂ -1.5 PNPs (a) before and (b) after 5 catalytic cycles. (c) XRD patterns before and after catalytic reactions.



Fig. S11 (a) Schematic illustration of the catalytic reduction reaction under NIR light irradation at 0.05 mg/ml and 3 W/cm². (b) Photoheating curve of MoS₂-1.5 PNPs. UV-vis absorption spectra of the reaction solution (c) without NaBH₄ or MoS₂-1.5 PNPs, and (d) when NaBH₄ was replaced by NaOH (0.5 mM) after irradiation for 15 min.



Fig. S12 UV-vis absorption spectra of the reduction of 4-Nip with MoS_2 -1.5 PNPs at 0.05 mg/ml and 3 W/cm² within 200 s.

Sample	MoS ₂ (%)	Carbon (%)
MoS ₂ -1 PNPs	63.3	36.7
MoS ₂ -1.5 PNPs	61.1	38.9
MoS ₂ -3 PNPs	69.2	30.8

Table S1 Mass fraction of carbon and MoS_2 in various particles.

Table S2 Specific surface area of various MoS₂ PNPs.

Sample	Specific surface area(m ² /g)
bulk MoS ₂	36.3
MoS ₂ -1 PNPs	139.9
MoS ₂ -1.5 PNPs	106.6
MoS ₂ -3 PNPs	81.6

Table S3 Summary of k_{app} of various MoS₂ PNPs.

Content		k_{app}	$_{pp}$ (s ⁻¹)	
(mg/mL)	bulk MoS ₂	MoS ₂ -1 PNPs	MoS ₂ -1.5 PNPs	MoS ₂ -3 PNPs
0.04	2.93×10 ⁻³ ±5.8×10 ⁻⁴	3.03×10 ⁻³ ±4.1×10 ⁻⁵	3.98×10 ⁻³ ±2.1×10 ⁻⁴	2.11×10 ⁻³ ±1.9×10 ⁻⁴
0.06	4.47×10 ⁻³ ±7.4×10 ⁻⁴	5.41×10 ⁻³ ±7.4×10 ⁻⁴	7.55×10 ⁻³ ±7.4×10 ⁻⁴	3.26×10 ⁻³ ±7.7×10 ⁻⁴
0.08	4.74×10 ⁻³ ±5.8×10 ⁻⁴	8.05×10 ⁻³ ±1.6×10 ⁻⁴	10.74×10 ⁻³ ±1.6×10 ⁻⁴	6.34×10 ⁻³ ±4.3×10 ⁻⁴
0.1	7.67×10 ⁻³ ±2.1×10 ⁻⁴	9.97×10 ⁻³ ±5.6×10 ⁻⁴	12.31×10 ⁻³ ±5.6×10 ⁻⁴	6.95×10 ⁻³ ±1.7×10 ⁻⁴

Table S4 Summary of k_{app} of MoS₂-1.5 PNPs in the presence/absence of NIR light illumination.

1/T (K ⁻¹)	k _{app} without NIR light (s ⁻¹)	1/T (K ⁻¹)	k _{app} with NIR light (s ⁻¹)
0.00333	4.43×10 ⁻³ ±2.31×10 ⁻⁴	0.00332	5.96×10 ⁻³ ±2.66×10 ⁻⁴
0.00330	5.11×10 ⁻³ ±2.03×10 ⁻⁴	0.00328	7.65×10 ⁻³ ±2.57×10 ⁻⁴
0.00327	5.43×10 ⁻³ ±6.02×10 ⁻⁴	0.00326	7.68×10 ⁻³ ±3.38×10 ⁻⁴
0.00325	6.66×10 ⁻³ ±3.61×10 ⁻⁴	0.00323	8.54×10 ⁻³ ±3.58×10 ⁻⁴
0.00321	7.66×10 ⁻³ ±2.04×10 ⁻⁴	0.00320	9.94×10 ⁻³ ±5.52×10 ⁻⁴