

Electronic Supplementary Information (ESI) for

Gold nanoparticles encapsulated in hierarchical porous polycarbazole: preparation and application in catalytic reduction

Jing Liu,^{a,b} Qi Chen,^{*,a} Ya-Nan Sun,^a Meng-Ying Xu,^a Wei Liu,^{*,b} and

Bao-Hang Han^{*,a}

^a *CAS Key Laboratory of Nanosystem and Hierarchical Fabrication, CAS Center for Excellence in Nanoscience, National Center for Nanoscience and Technology, Beijing 100190, China*

^b *University of Chinese Academy of Sciences, Beijing 100049, China*

Tel: +86 10 8254 5576. Email: hanbh@nanoctr.cn

Tel: +86 10 8825 6980. Email: weiliu@ucas.ac.cn

Tel: +86 10 8254 5708. Email: chenq@nanoctr.cn

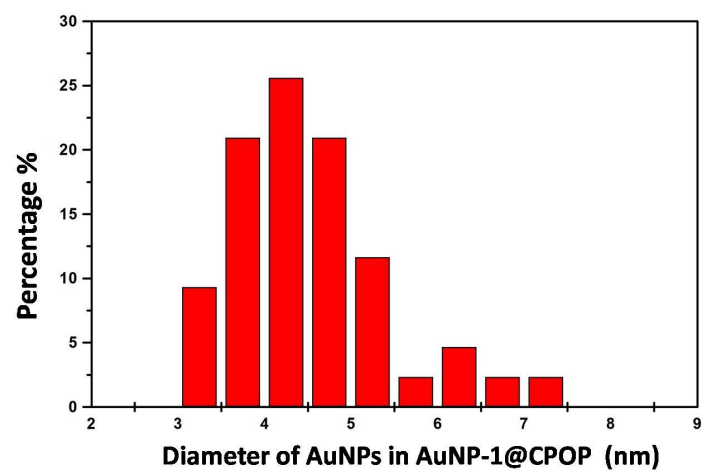


Fig. S1. The size distribution of AuNPs in AuNP-1@CPOP.

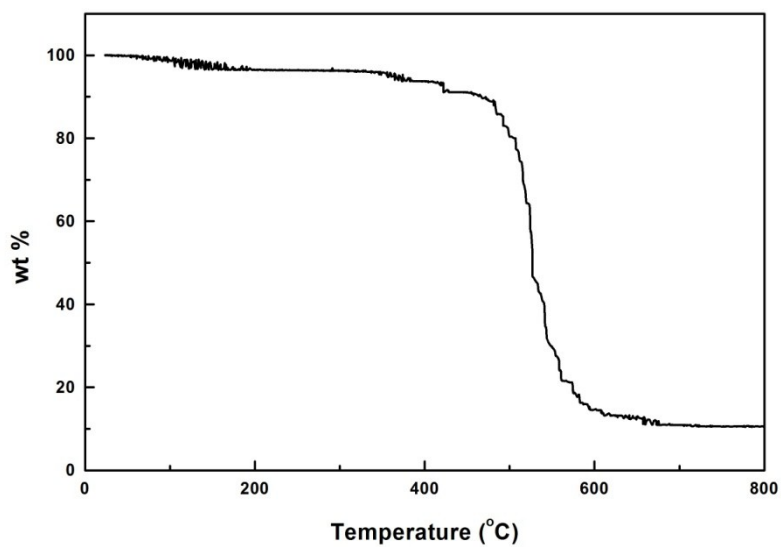


Fig. S2. TGA curve of AuNP-1@CPOP in the air.

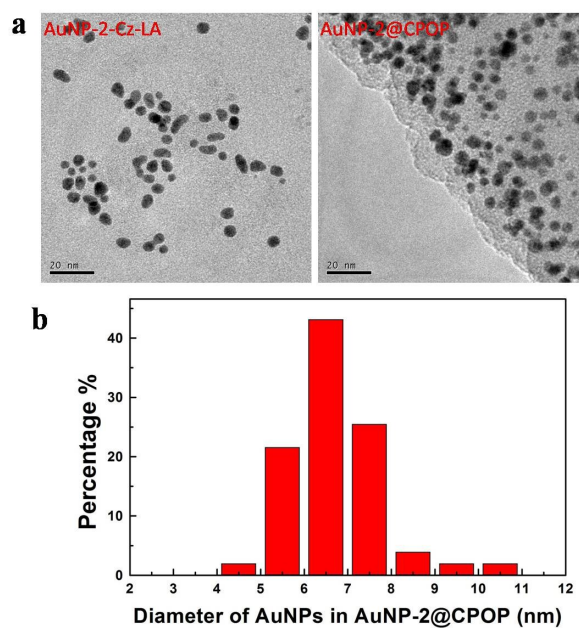


Fig.S3. a) TEM images of AuNP-2-Cz-LA, AuNP-2@CPOP. b) Size distribution of AuNPs in AuNP-2@CPOP.

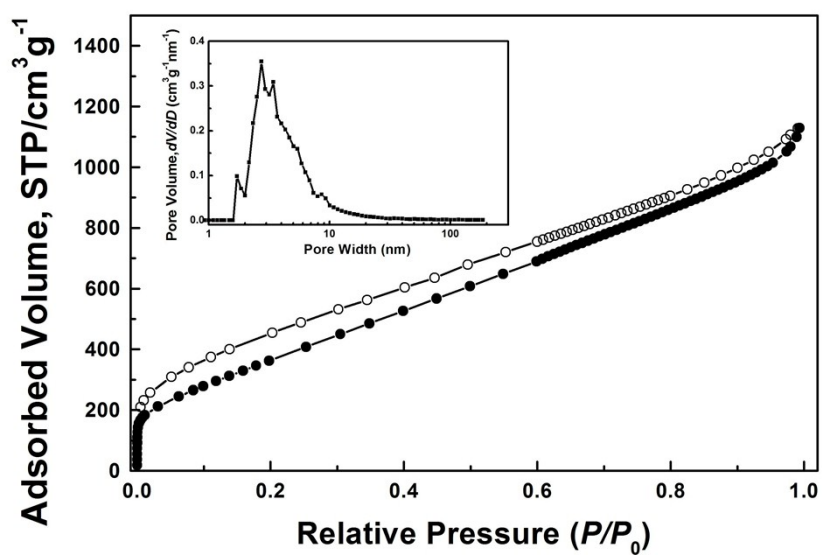


Fig.S4. Nitrogen adsorption-desorption isotherm of AuNP-2@CPOP at 77 K and the inset PSD profile calculated by NLDFT (the adsorption and desorption branches are labeled with solid and open dot, respectively).

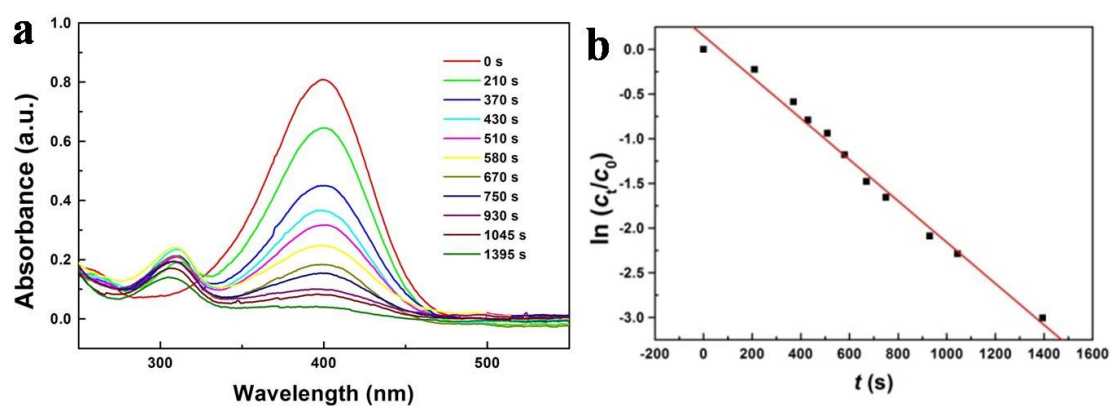


Fig. S5. a) Time-dependent normalized absorption spectra of 4-nitrophenol reduced by NaBH₄ in the presence of AuNP-2@CPOP. b) Plot of $\ln(c_t/c_0)$ against the reaction time t .

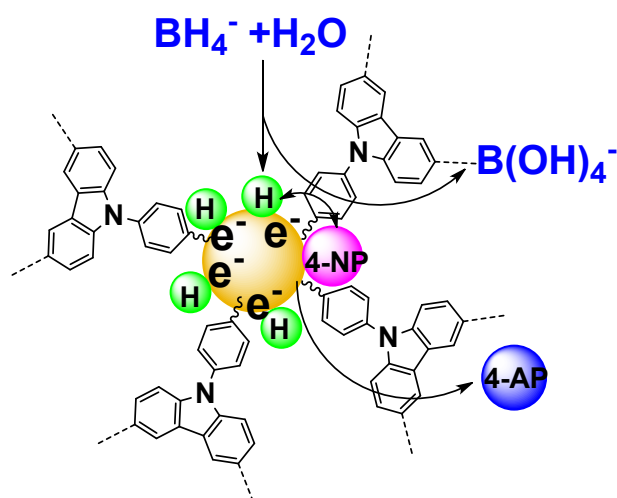


Fig. S6. The possible schematic mechanism for catalytic reduction of 4-nitrophenol by AuNPs@CPOP in the presence of NaBH₄.

Table S1. Porosity properties of AuNPs@CPOP.

Polymer	S_{BET}^a	S_{Langmuir}^b	S_{micro}^c	V_{total}^d	D_{pore}^e
	(m ² g ⁻¹)	(m ² g ⁻¹)	(m ² g ⁻¹)	(cm ³ g ⁻¹)	(nm)
AuNP-1@CPOP	930	1260	300	0.799	2.0–10.8
AuNP-2@CPOP	1460	1590	760	0.564	1.7–12.7

^a Use the BET method to calculate specific surface area from the nitrogen adsorption–desorption isotherm.

^b Apply the Langmuir equation to calculate specific surface area from the nitrogen adsorption isotherm.

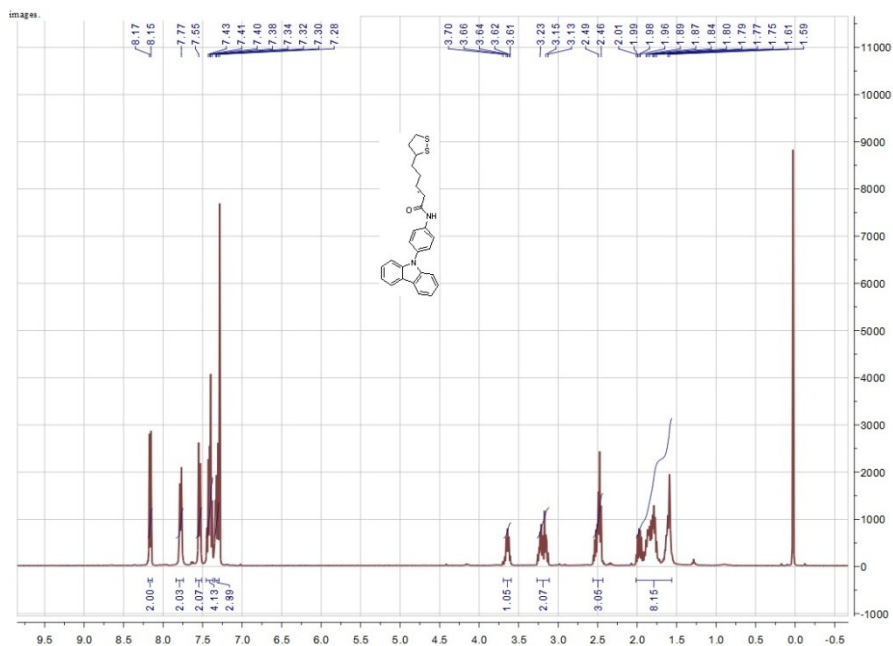
^c Use the *t*-plot method to calculate micropore surface area from the nitrogen adsorption isotherm.

^d Total pore volume at $P/P_0 = 0.97$.

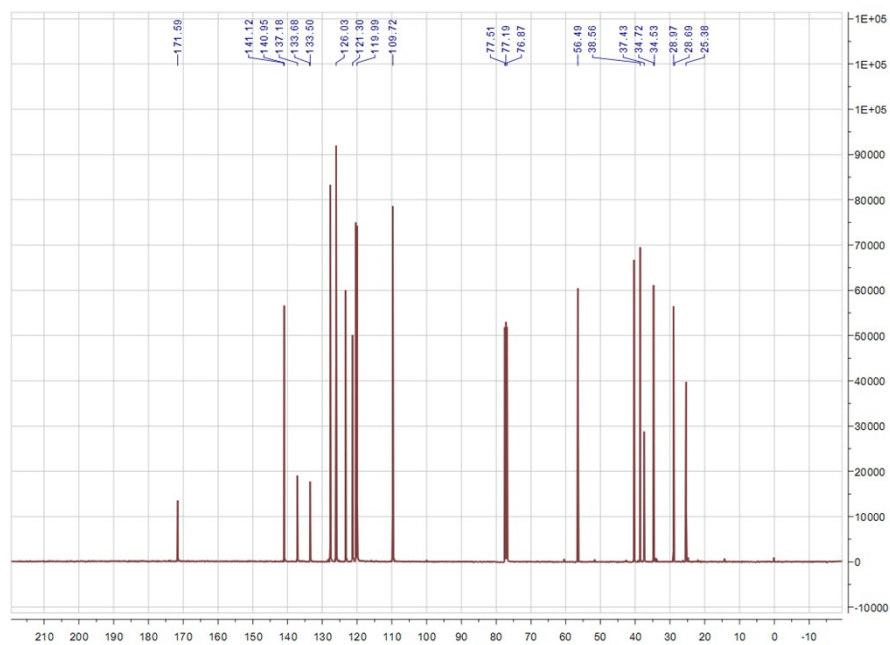
^e Use the nonlocal density function theory (NLDFIT) method to calculate data from nitrogen adsorption isotherms and pore diameter is dominant.

Table S2. Synthesis of AuNPs with different sizes and related catalytic behaviors of corresponding polymers in reduction.

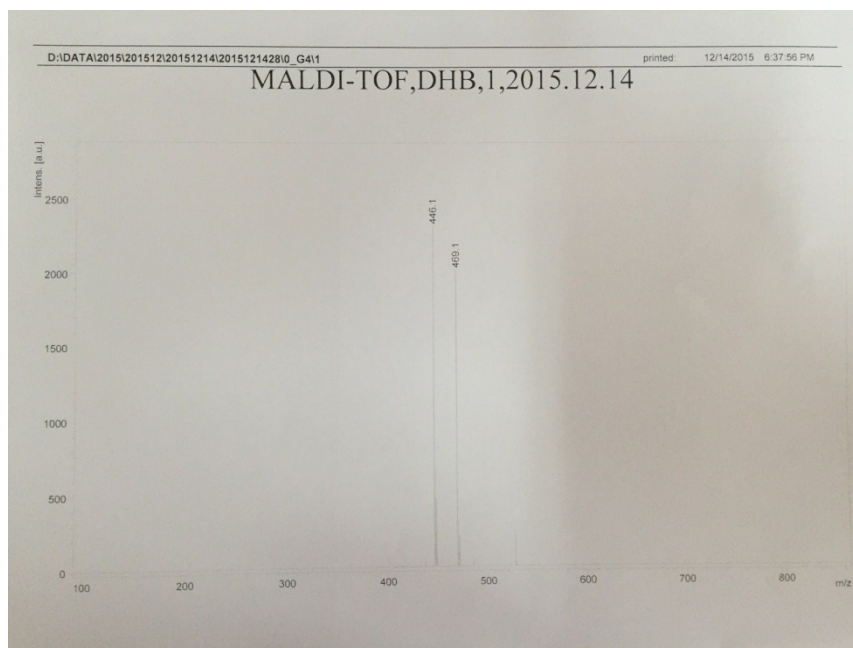
Polymer	HAuCl ₄ •4H ₂ O (mg)	Cz-LA (mg)	NaBH ₄ (mg)	Size of AuNPs (nm)	k_{app} ($\times 10^{-3} \text{ s}^{-1}$)	κ ($\text{s}^{-1} \text{ g}^{-1}$)
AuNP-1@CPOP	160	28	230	4.5 $\pm$ 1.5	4.04	17.57
AuNP-2@CPOP	160	10	25	6.5 $\pm$ 1.5	2.31	10.04



¹H NMR of Cz-LA.



¹³C NMR of Cz-LA.



Mass Spectrum of Cz-LA.