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

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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 NaBH$_4$ 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 NaBH$_4$. 
Table S1. Porosity properties of AuNPs@CPOP.

<table>
<thead>
<tr>
<th>Polymer</th>
<th>( S_{\text{BET}} ) (^a) (m(^2) g(^{-1}))</th>
<th>( S_{\text{Langmuir}} ) (^b) (m(^2) g(^{-1}))</th>
<th>( S_{\text{micro}} ) (^c) (m(^2) g(^{-1}))</th>
<th>( V_{\text{total}} ) (^d) (cm(^3) g(^{-1}))</th>
<th>( D_{\text{pore}} ) (^e) (nm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>AuNP-1@CPOP</td>
<td>930</td>
<td>1260</td>
<td>300</td>
<td>0.799</td>
<td>2.0–10.8</td>
</tr>
<tr>
<td>AuNP-2@CPOP</td>
<td>1460</td>
<td>1590</td>
<td>760</td>
<td>0.564</td>
<td>1.7–12.7</td>
</tr>
</tbody>
</table>

\(^a\) 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 (NLDFT) 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.

<table>
<thead>
<tr>
<th>Polymer</th>
<th>HAuCl₄•4H₂O (mg)</th>
<th>Cz-LA (mg)</th>
<th>NaBH₄ (mg)</th>
<th>Size of AuNPs (nm)</th>
<th>k&lt;sub&gt;app&lt;/sub&gt; (×10⁻³ s⁻¹)</th>
<th>κ (s⁻¹ g⁻¹)</th>
</tr>
</thead>
<tbody>
<tr>
<td>AuNP-1@CPOP</td>
<td>160</td>
<td>28</td>
<td>230</td>
<td>4.5±1.5</td>
<td>4.04</td>
<td>17.57</td>
</tr>
<tr>
<td>AuNP-2@CPOP</td>
<td>160</td>
<td>10</td>
<td>25</td>
<td>6.5±1.5</td>
<td>2.31</td>
<td>10.04</td>
</tr>
</tbody>
</table>
\(^1\)H NMR of Cz-LA.

\(^{13}\)C NMR of Cz-LA.
Mass Spectrum of Cz-LA.