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## **Supporting Information**

### **Diaminotetrazine Based Mesoporous C<sub>3</sub>N<sub>6</sub> with Well-Ordered 3D Cubic Structure and its Excellent Photocatalytic Performance on Hydrogen Evolution**

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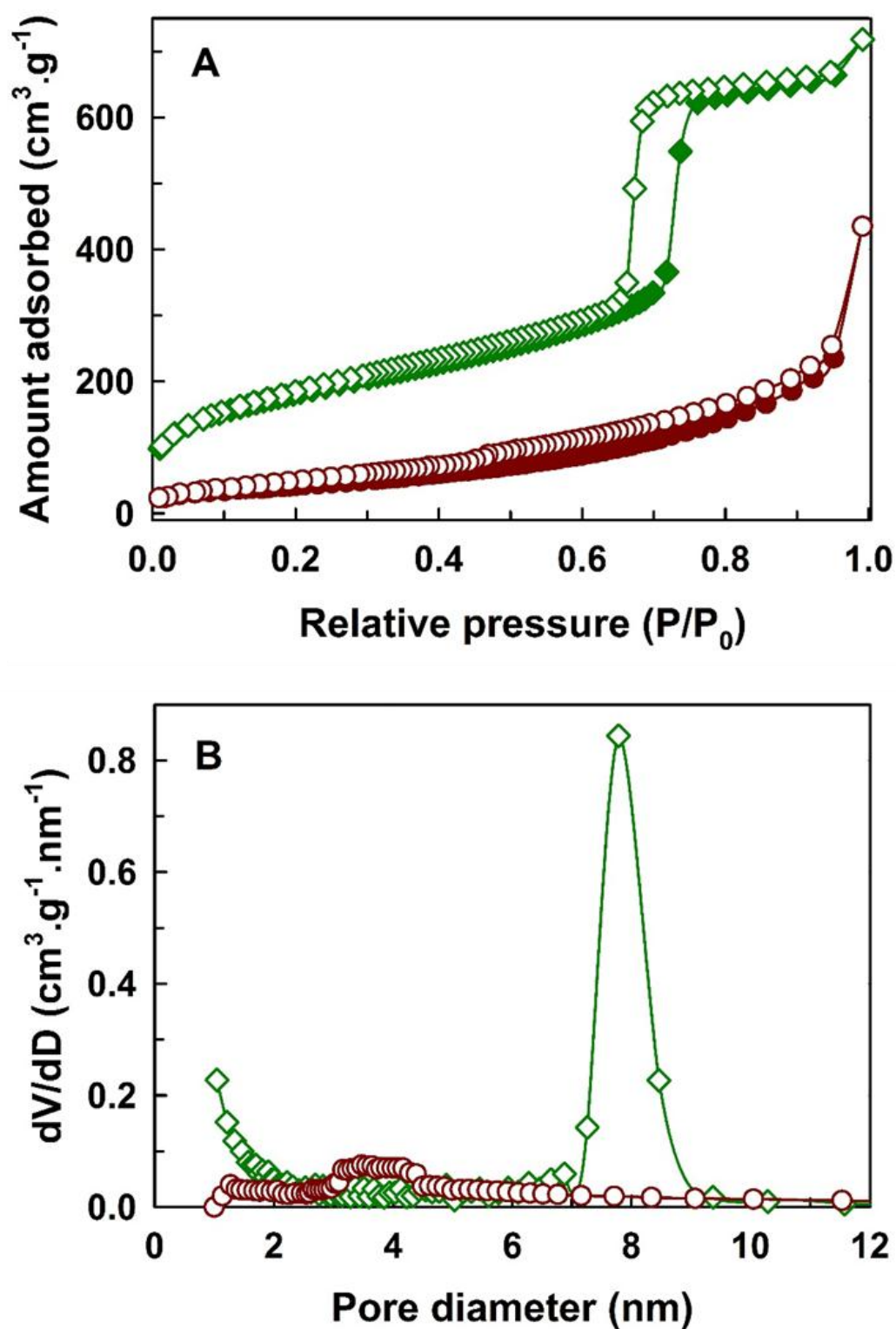
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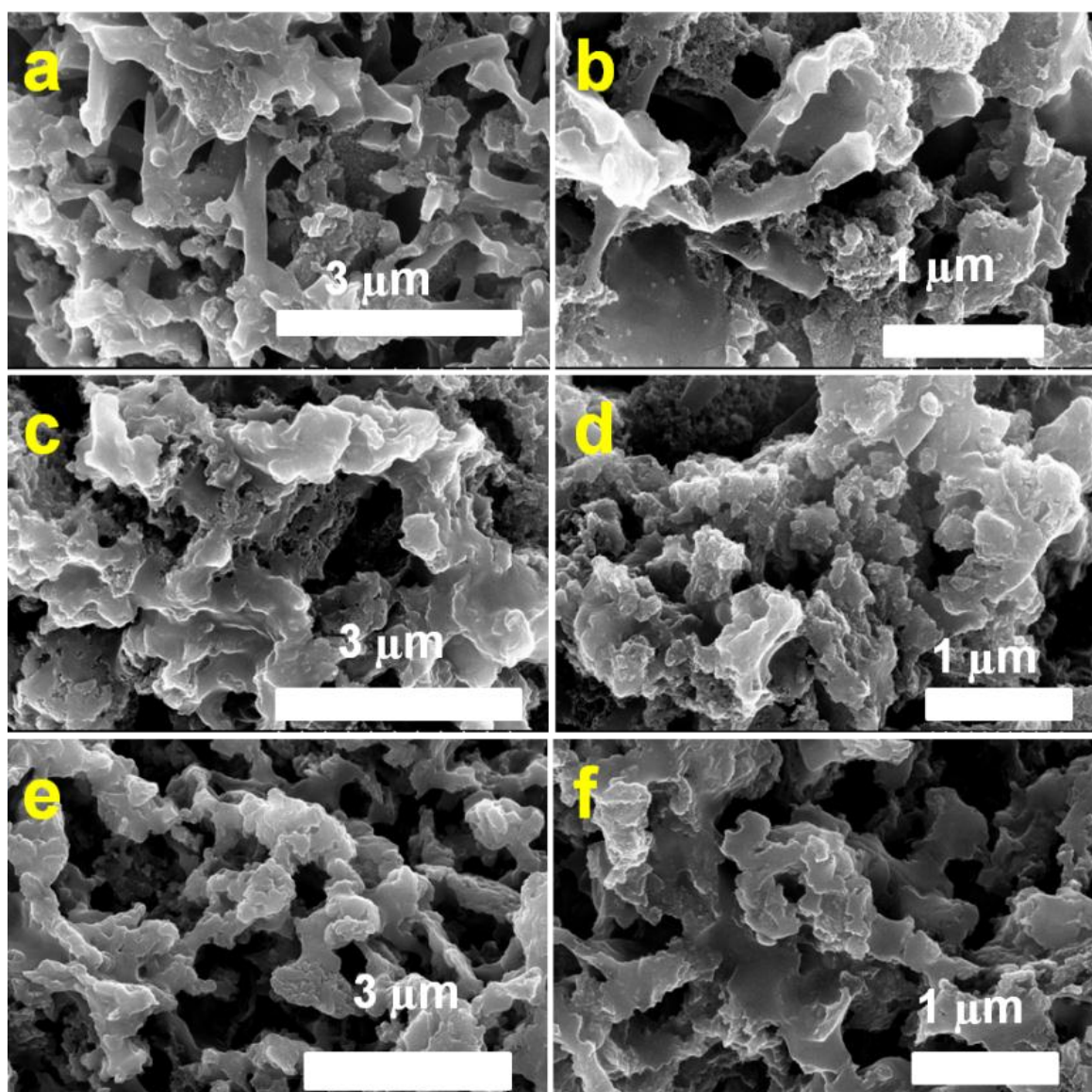
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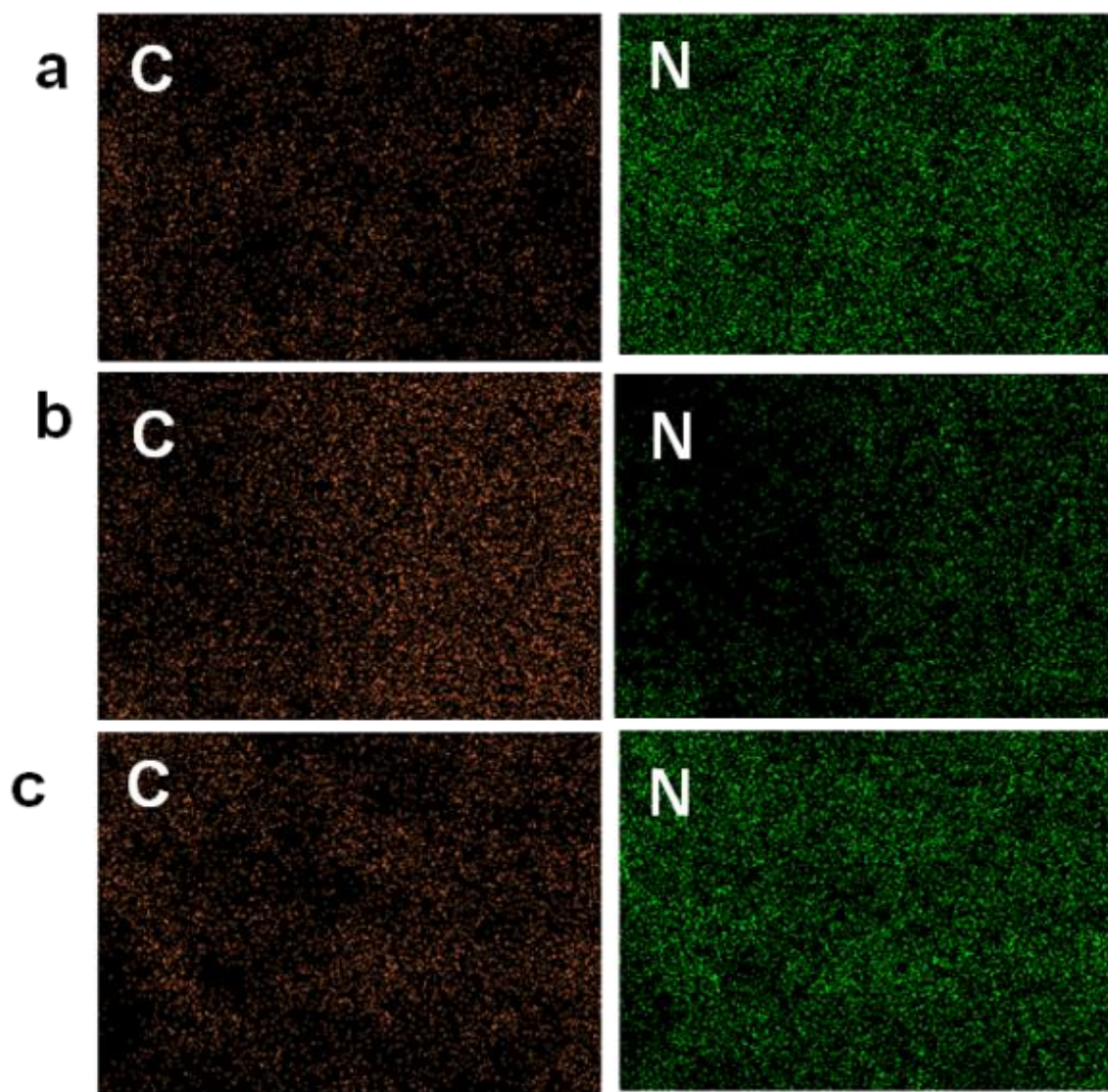
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**Figure S1.** (A) Nitrogen adsorption–desorption isotherms and (B) BJH pore-size distributions of c-MCN-100 (circles) and KIT-6-100 (diamonds) silica template.

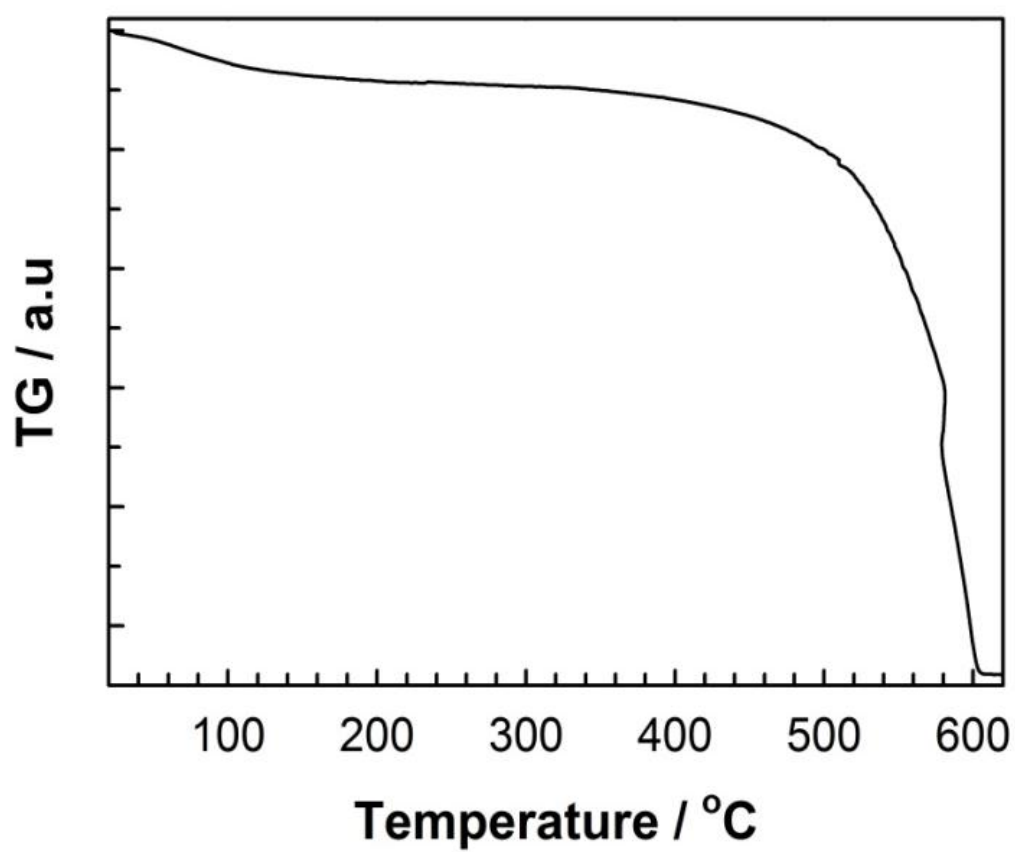


**Figure S2.** HRSEM images of (a-b) c-MCN-100, (c-d) c-MCN-130 and (e-f) c-MCN-150 samples at different magnifications.



**Figure S3.** Elemental mappings of (a) c-MCN-100, (b) c-MCN-130 and (c) c-MCN-150.

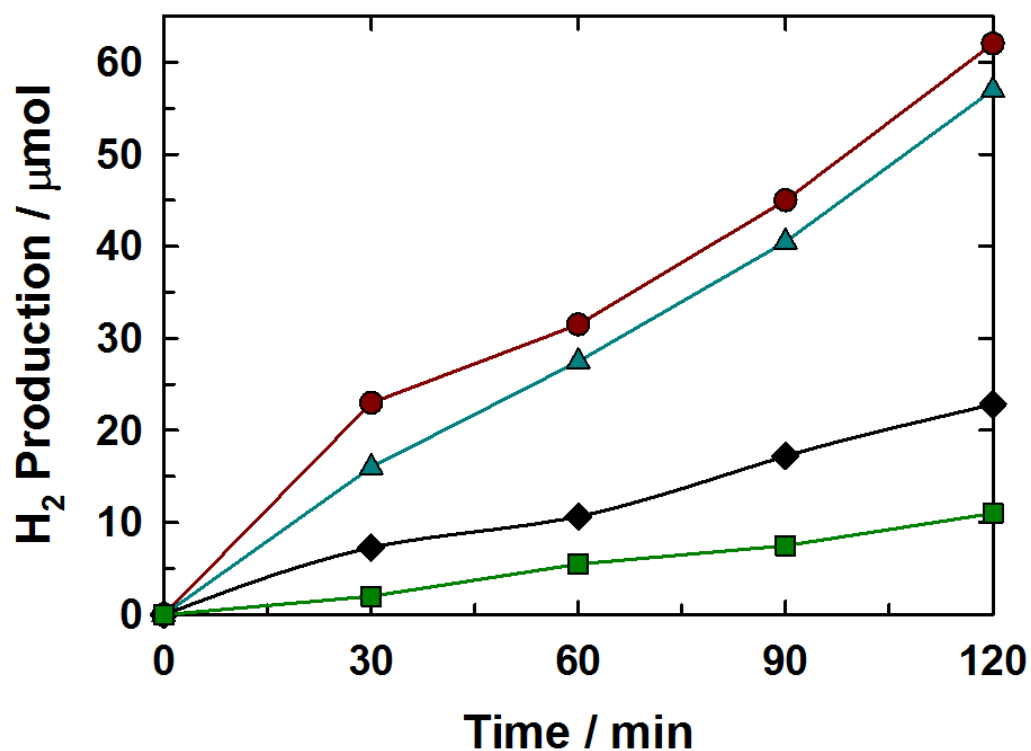




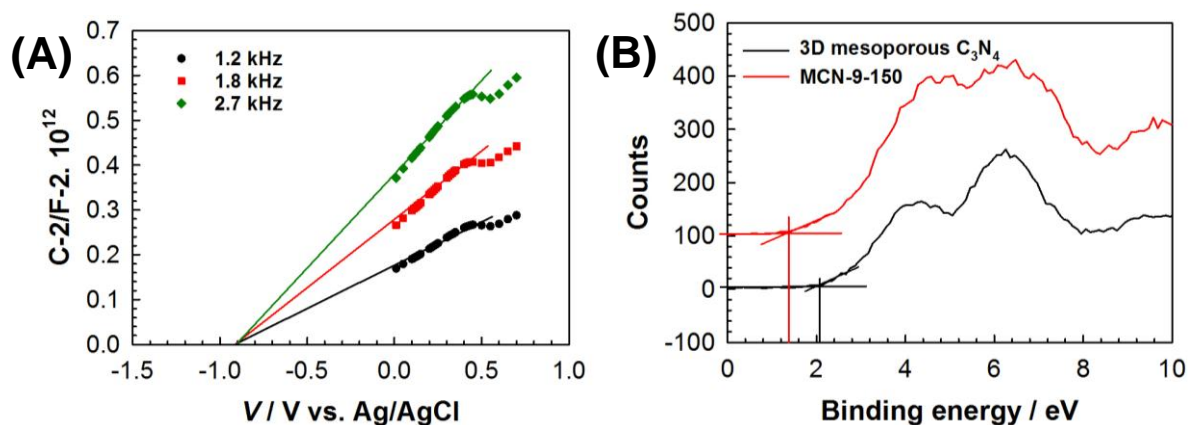
**Figure S4.** TG curve of c-MCN-150 under nitrogen atmosphere.

**Table S1** Textural parameters of KIT-6 silica templates having different pore diameters synthesized at 100, 130 and 150°C temperatures

	$d_{(211)}$ Spacing	Unit cell	$A_{\text{BET}}$	$V_p$	$d_{p, \text{BJH}}$
Material	(nm)	$a_0$ (nm)	( $\text{m}^2 \cdot \text{g}^{-1}$ )	( $\text{cm}^3 \cdot \text{g}^{-1}$ )	(nm)
KIT-6-100	9.17	22.5	728	0.99	8.0
KIT-6-130	9.62	23.6	625	1.32	9.9
KIT-6-150	9.81	24.0	555	1.53	11.3



**Figure S5.** Time course of H<sub>2</sub> gas evolution using MCN-9 photocatalyst (circles) as a function of time, with reference to mesoporous C<sub>3</sub>N<sub>6</sub> with 2D structure (up triangles), 3D mesoporous C<sub>3</sub>N<sub>4</sub> and bulk non-porous C<sub>3</sub>N<sub>4</sub>.



**Figure S6.** (A) Electrochemical Mott-Schottky plots of MCN-9-150 at different frequencies (B) XPS valence band spectra of 3D mesoporous C<sub>3</sub>N<sub>4</sub> and MCN-9-150.

**Table S2** The apparent quantum efficiency (AQE) for photocatalytic hydrogen evolution over MCN-9, mesoporous  $C_3N_6$  with 2D structure, bulk non-porous  $C_3N_6$ , 3D mesoporous  $C_3N_4$  and bulk non-porous  $C_3N_4$  photocatalysts, using diode laser as the incident light (405 nm)

Sample name	AQE (%)
MCN-9-150	0.212
mesoporous $C_3N_6$ with 2D structure	0.185
bulk non-porous $C_3N_6$	0.037
3D mesoporous $C_3N_4$	0.071
bulk non-porous $C_3N_4$	0.037