

Electronic Supporting Information:

Iron-based nanoparticles embedded in graphitic layer of carbon architectures as stable heterogeneous Friedel-Crafts acylation catalysts

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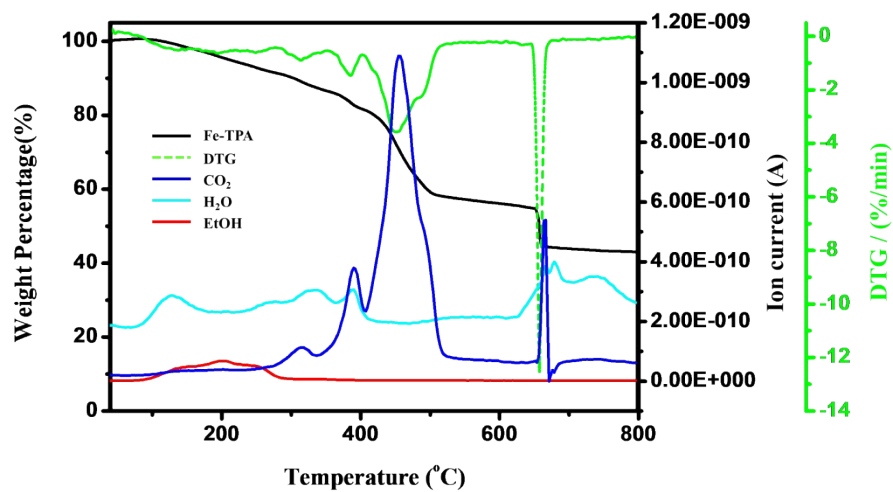


Fig. S1 TG-MS profiles of the Fe-TPA under inert atmosphere.

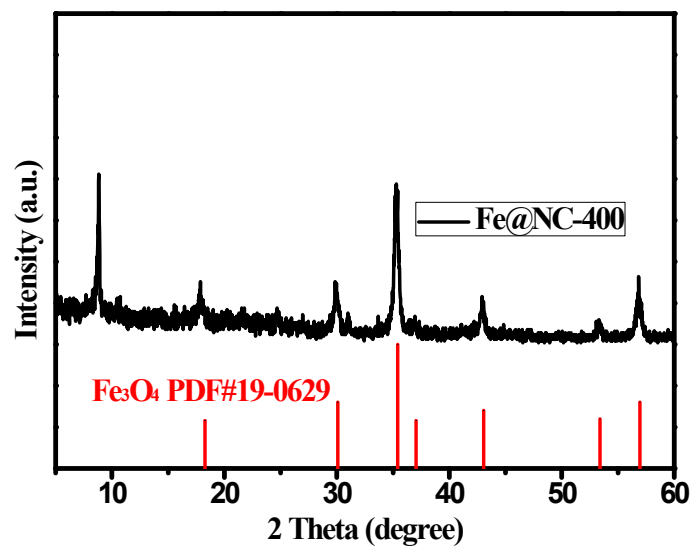


Fig. S2 XRD pattern of Fe@NC-400.

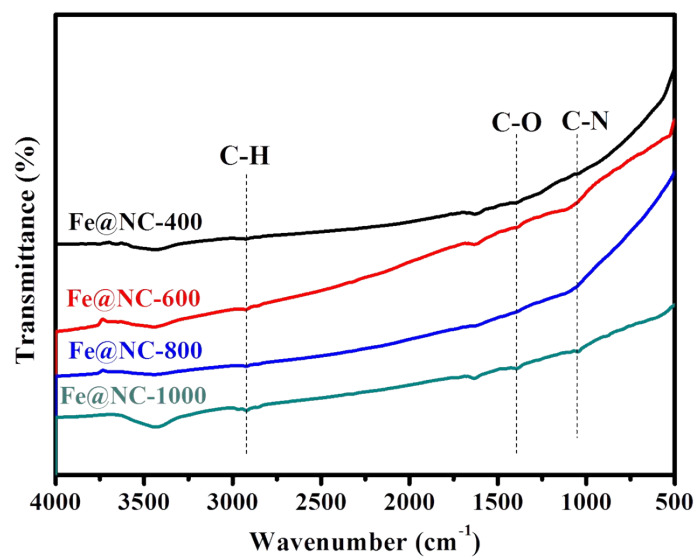


Fig. S3 FT-IR spectra of the Fe@NC-*T* catalysts.

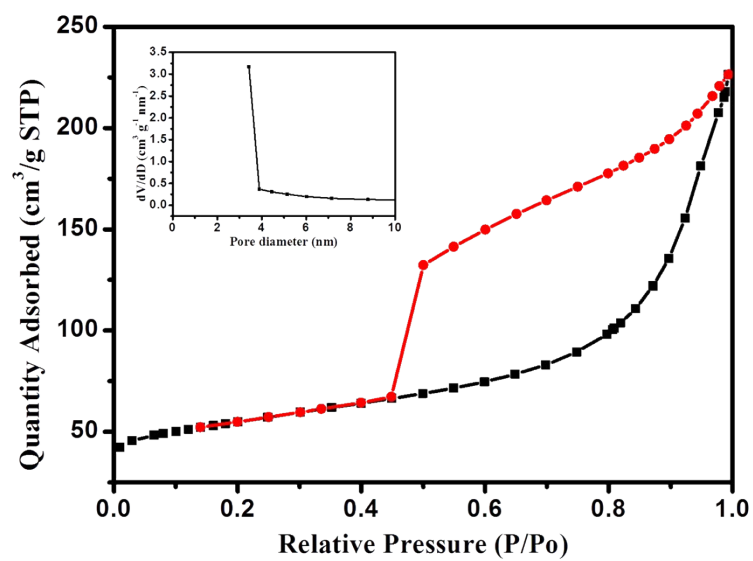


Fig. S4 Nitrogen isothermal adsorption-desorption curves for Fe@C-800. Inset: pore size distribution profile based on the DFT model.

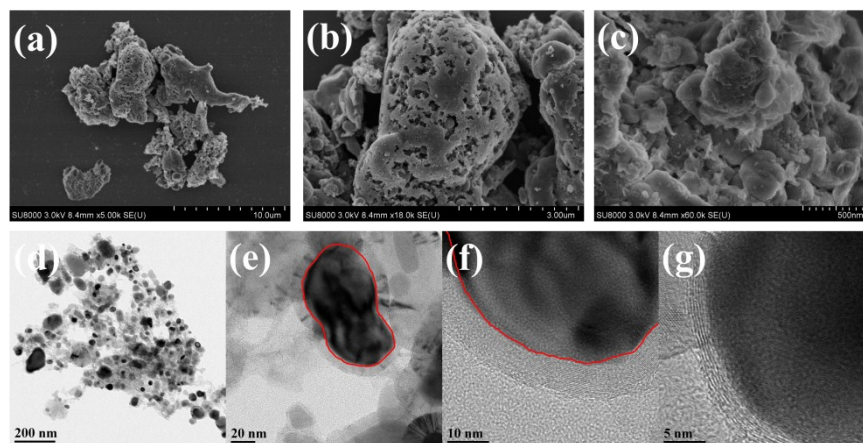


Fig. S5 (a-c) SEM and (d-g) TEM/HRTEM images of Fe@NC-800.

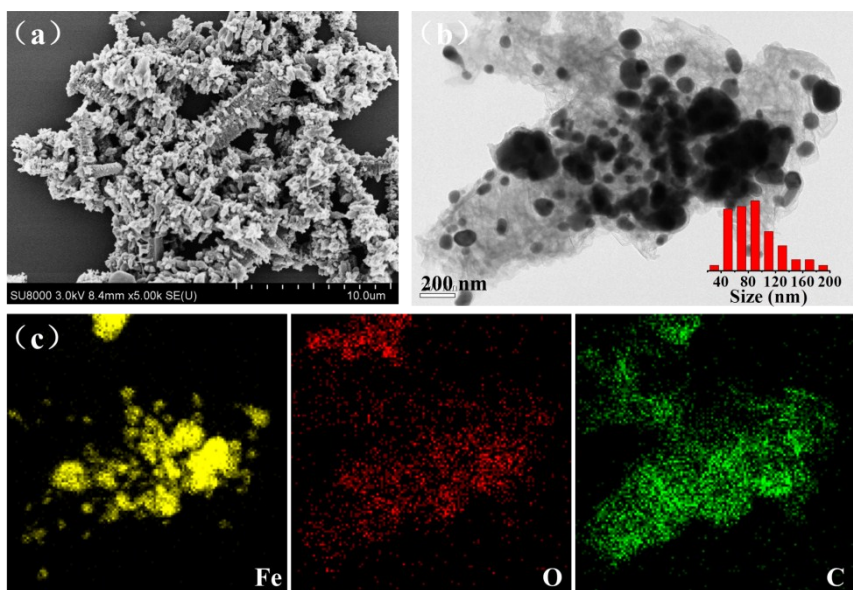


Fig. S6 (a) SEM and (b) TEM images of Fe@C-800. (c) Elemental mapping revealing the elemental distribution.

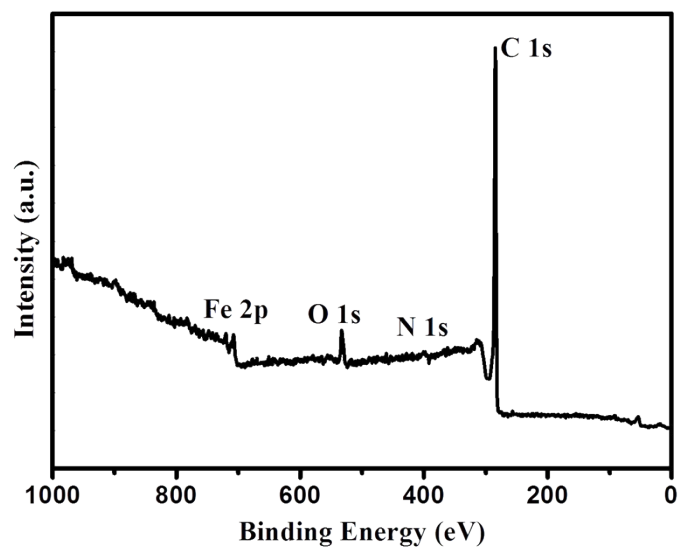


Fig. S7 XPS survey spectra of Fe@NC-800.

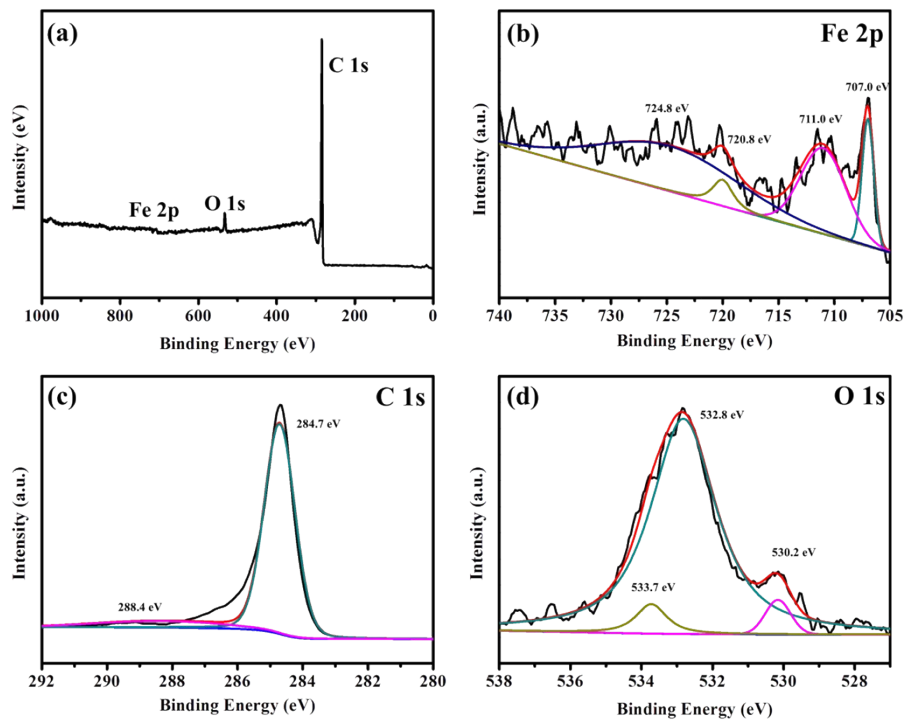


Fig. S8 XPS survey spectra of (a) Fe@C-800, (b) Fe 2p, (c) C 1s and (d) O 1s of Fe@C-800.

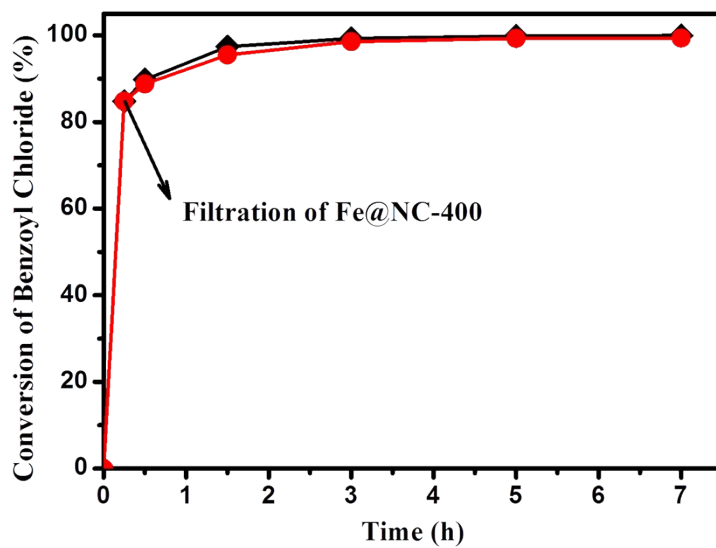


Fig. S9 Friedel-Crafts acylation property over (◆) Fe@NC-400 and the leaching test (●). Reaction conditions: 130 °C reaction temperature; 20 mmol m-xylene, 10 mmol benzoyl chloride, and 10 mmol dodecane; 50 mg catalyst.

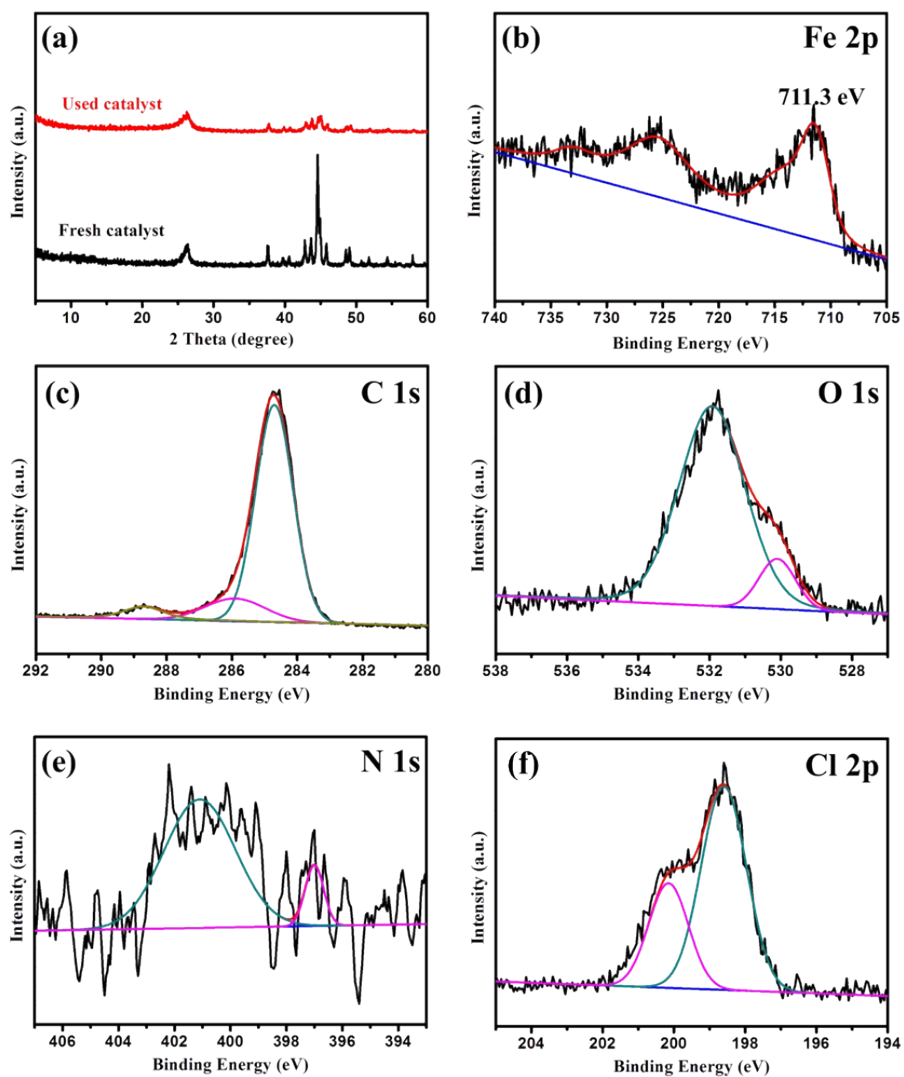


Fig. S10 (a) XRD diffraction patterns of fresh and used Fe@NC-800 catalysts after five consecutive cycles; and XPS survey spectra of (b) Fe 2p, (c) C 1s, (d) O 1s, (e) N 1s and (f) Cl 2p of the used Fe@NC-800 catalyst.

Table S1 Summary of the porous properties of Fe@NC-*T* and Fe@C-800 catalysts.

	S_{BET}^a (m ² g ⁻¹)	S_{micro}^b (m ² g ⁻¹)	S_{meso}^c (m ² g ⁻¹)	V_{pore}^d (cm ³ g ⁻¹)
Fe@NC-600	232	147	85	0.24
Fe@NC-800	174	51	123	0.35
Fe@NC-1000	119	39	80	0.26
Fe@C-800	180	75	105	0.32

^a Calculated via the BET method.

^b Calculated via the t-plot method.

^c $S_{\text{meso}} = S_{\text{BET}} - S_{\text{micro}}$.

^d Calculated based on the N₂ adsorption at $p/p_0 = 0.99$.

Table S2 The element compositions of various samples determined from a PerkinElmer 2400 CHN elemental analyzer and ICP-AES.

Samples	Element analysis				
	C (wt %)	H (wt %)	N (wt %)	O (wt %)	Fe (wt %)
Fe-TPA	39.14	3.24	-	40.76	16.86
Fe-DABCO-TPA	53.59	5.25	7.00	27.33	6.83
Fe@C-800	27.57	0.30	-	12.51	59.62
Fe@NC-800	50.92	0.43	0.51	2.74	45.40
Fe@NC-800*					44.74

* The used Fe@NC-800 catalyst after FCA reactions.

Table S3 The elemental contents on the surface of Fe@NC-800 obtained from XPS.

Samples	Elemental composition (At. %)				
	C 1s	O 1s	Fe 2p	N 1s	Cl 2p
Fe@C-800	94.75	4.81	0.44	-	-
Fe@NC-800	84.56	10.40	1.08	3.97	-
Fe@NC-800*	85.06	5.55	1.27	2.68	5.44

* The used Fe@NC-800 catalyst after FCA reactions.