Electronic Supplementary Information

Controllable synthesis of carbon encapsulated iron phosphide nanoparticles for chemoselective hydrogenation of aromatic nitroarenes to anilines

Yanan Zhu,[a, b] Shuliang Yang,[a] Changyan Cao,*[a, b] Weiguo Song,*[a, b] and Li-Jun Wan[a]

[a]Beijing National Laboratory for Molecular Sciences, Laboratory of Molecular Nanostructures and Nanotechnology, CAS Research/Education Center for Excellence in Molecular Sciences, Institute of Chemistry, Chinese Academy of Sciences, Beijing, 100190, P.R. China.

[b] University of Chinese Academy of Sciences, Beijing, 100049, P.R. China.

E-mail: cycao@iccas.ac.cn, wsong@iccas.ac.cn.

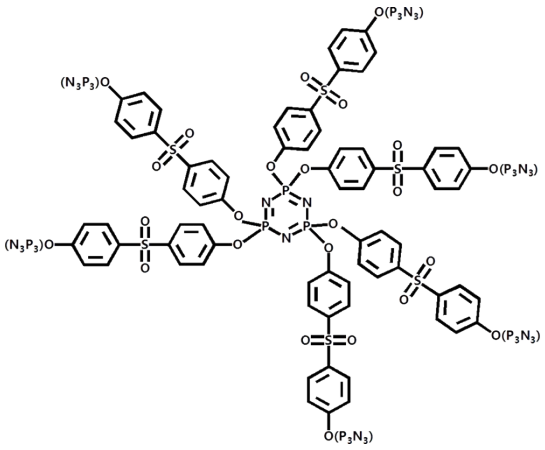


Fig. S1 Molecular structure of PZS

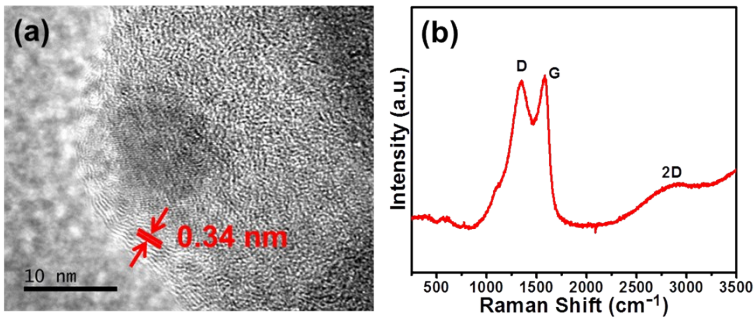


Fig. S2 (a) HRTEM image and (b) Raman spectra of Fe_2P@C

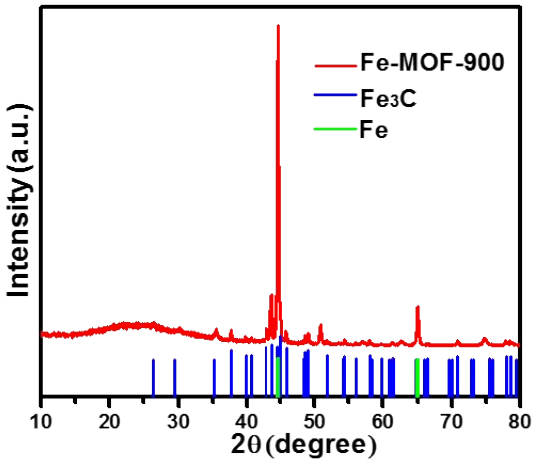


Fig. S3 XRD pattern of Fe-MOF-900.

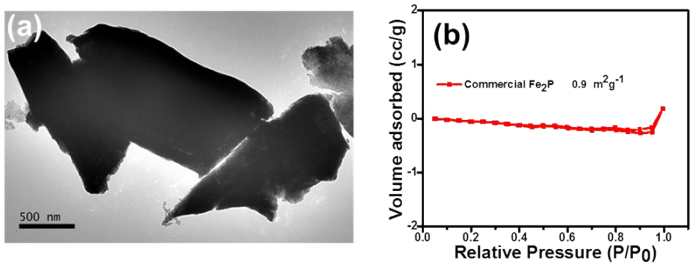


Fig. S4 TEM image and N_2 adsorption-desorption isotherm of commercial Fe_2P.

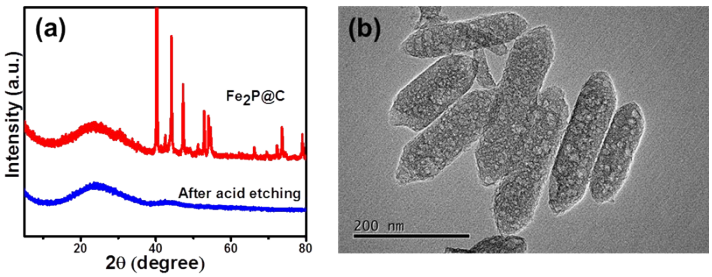


Fig. S5 XRD pattern (a) and TEM image (b) of Fe_2P@C after etching with aqua regia for two days.

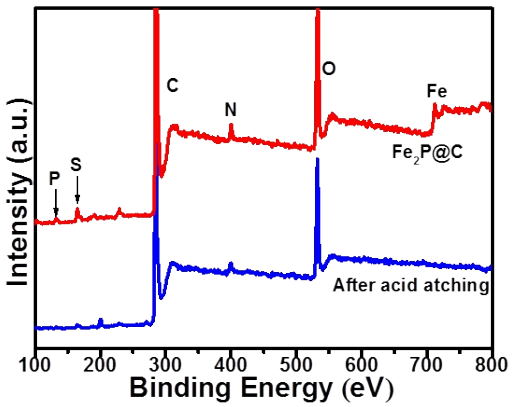


Fig. S6 XPS full spectrum of Fe_2P@C and after etching with aqua regia for two days.

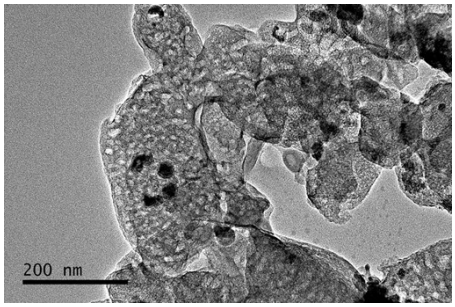


Fig. S7 TEM image of Fe_2P@C after reused for five times

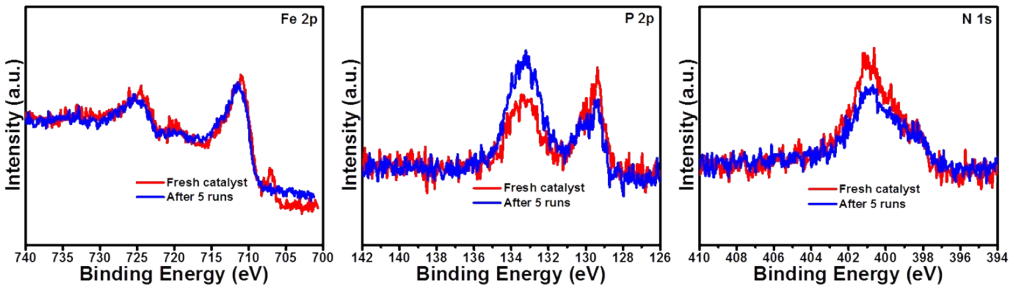
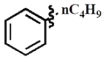
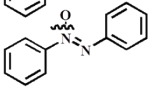
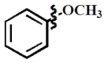


Fig. S8 XPS spectra of (a) Fe 2p, (b) P 2p and (c) N 1s of fresh catalyst (red lines) and after 5 runs (blue lines).

Table S1. The bond energy of the substituent groups

Bond energy (KJ/mol)		Bond energy (KJ/mol)	
	391.5±8		420.9±4.2
	309.4±3.5		416.7±5.9
	399.6±6.3		463.6±4.2
	463.6±4.2	C=O	728
C=C	611		