Electronic Supplementary Material (ESI) for Catalysis Science & Technology.

Highly active electron-deficient Pd clusters on N-doped active carbon for the hydrogenation of aromatic ring†

Renfeng Nie*, Hezhan Jiang, Xinhuan Lu, Dan Zhou and Qinghua Xia*

Table S1 Chemical compositions of N-doped AC obtained by XPS and elemental analyses.

Sample		400N-AC	600N-AC	800N-AC	1000N-AC	AC
XPS	at.% C	78.1	89.6	91.1	90.0	93.5
	at.% N	9.1	3.4	2.9	1.5	0
Elemental analysis	at.% C	76.6	82.7	84.1	87.1	93.4
	at.% N	7.3	2.0	1.8	0.7	0

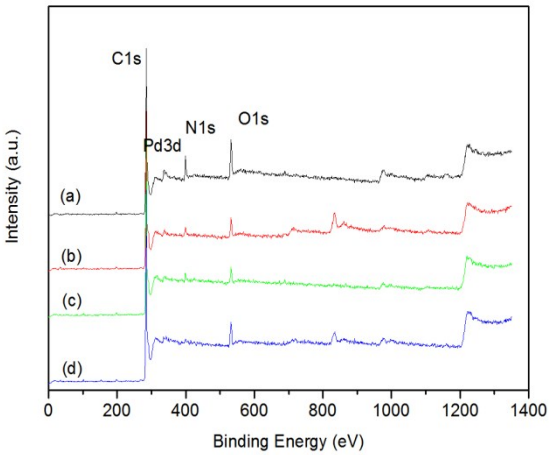

Fig. S1 XPS survey spectra of (a) Pd/400N-AC, (b) Pd/600N-AC, (c) Pd/800N-AC and (d) Pd/1000N-AC.

Table S2. Structural properties of N-doped carbon supported Pd catalysts.

Catalysts	S_{BET} (m^2/g)	V_P (cm^3/g)	D_p (nm)
Pd/AC	759	0.46	4.0
Pd/400N-AC	531	0.38	4.3
Pd/600N-AC	587	0.40	4.3
Pd/800N-AC	696	0.44	4.1
Pd/1000N-AC	747	0.45	4.0

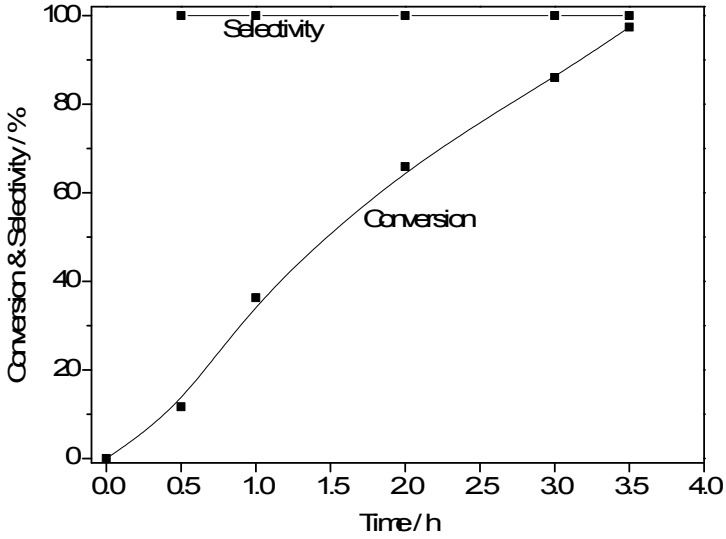

Fig. S2 Hydrogenation of benzoic acid catalyzed by Pd/800N-AC. Reaction conditions: 0.5 mmol BA, 20 mg catalyst (Pd (0.94 mol % to substrate)), 5 mL H_2O, 2.5 MPa H_2.

Table S3 Gram-scale transformation of BA on Pd/800N-AC.

Catalysts	t (h)	T (°C)	yield (%)	TOF (h^{-1})[c]
Pd/800N-AC	12	150	92.4	583.9

[a] Reaction conditions: 1.0 g BA, 55 mg catalyst , 25 mL H_2O, 2.5 MPa H_2.

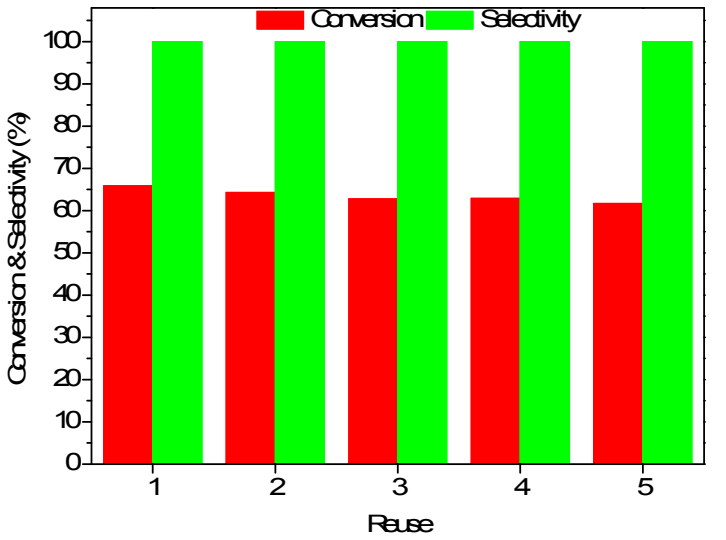

Fig. S3 Re-uses of Pd/800N-AC catalyst for the BA hydrogenation.
Reaction conditions: 0.5 mmol BA, catalyst 20 mg (Pd (0.94 mol % to substrate)), 5 mL H_2O, 2.5 MPa H_2, 2 h.

Table S4 Hydrogenation of benzoic acid over Pd/800N-AC catalyst in different solvents.[a]

Entry	Solvents	t (h)	T (^{o}C)	yield (%)
1	H_2O	2	110	65.9
2	THF	2	110	21.3
3	Cyclohexane	2	110	5.8
4	Ethanol	2	110	2.9

[a] Reaction conditions: 0.5 mmol BA, catalyst 20 mg (Pd (0.94 mol % to substrate)), 5 mL solvent,