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

Supporting Information

Constructing green mercury-free catalysts with single pyridinic N species for acetylene hydrochlorination and mechanism investigation

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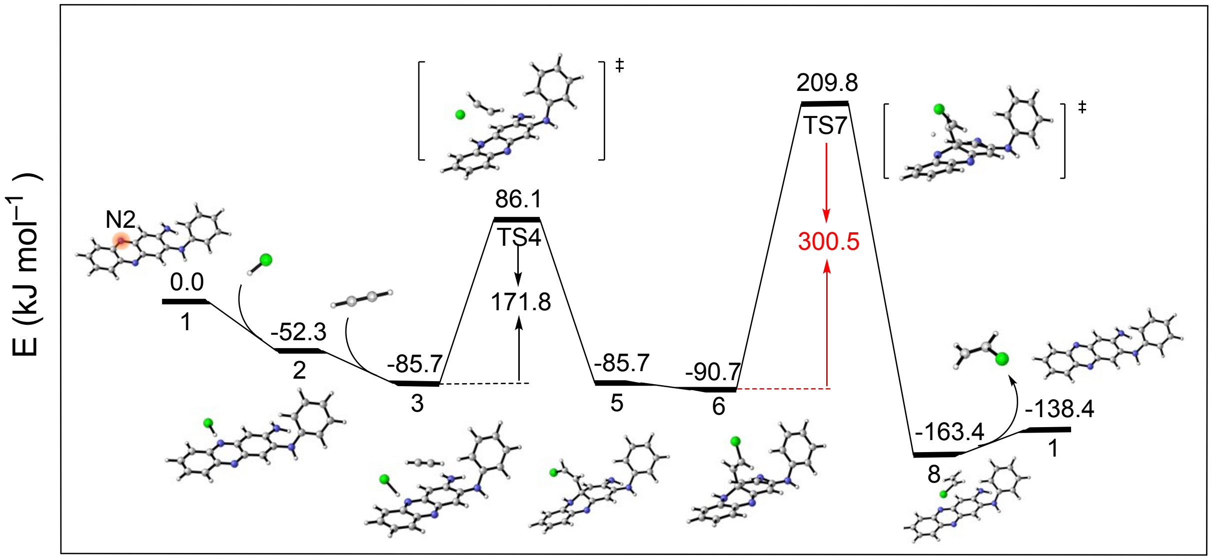

Fig. S1 Reaction energy diagram of the substances involved in the reaction path 2.

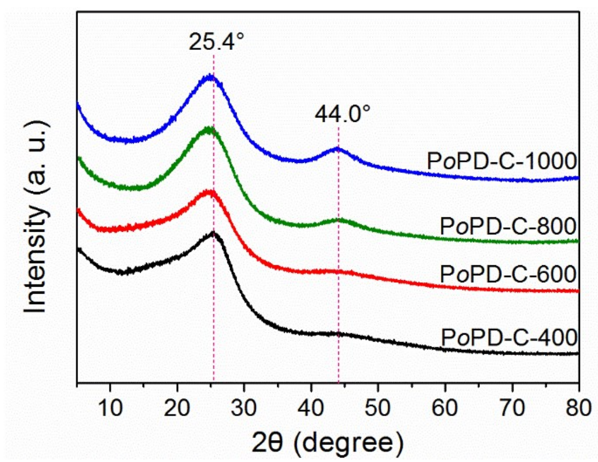

Fig. S2 XRD patterns of PoPD and PoPD-derived carbon materials.

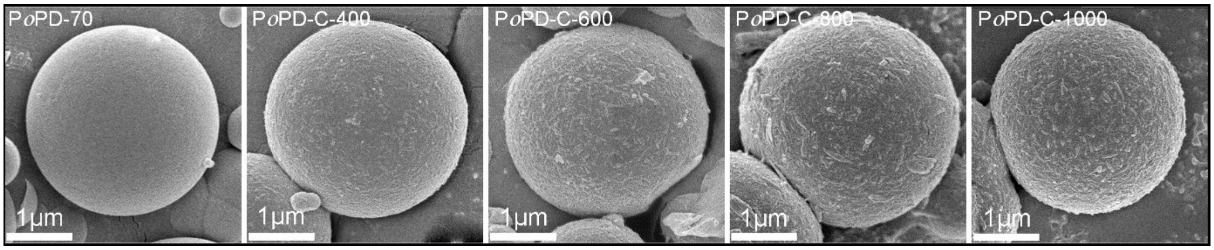

Fig. S3 SEM images of PoPD-derived carbon materials.

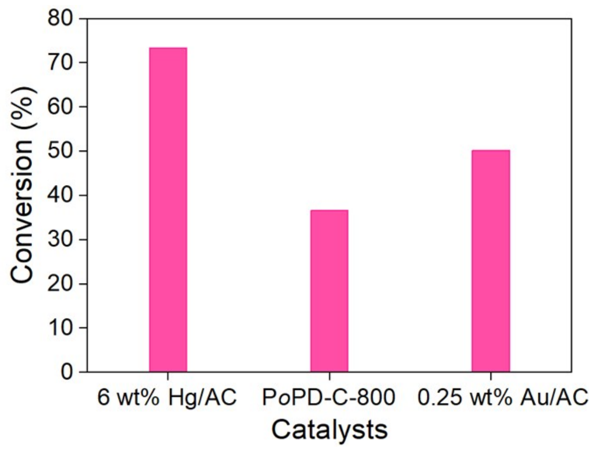

Fig. S4 Conversion of acetylene over 6 wt% Hg/C, PoPD-C-800, and 0.25 wt% Au/AC catalysts under 200 h^{-1} and 150 °C.

Table S1 Compositions of C, N, and O (wt %) in samples determined by XPS[a] and EA[b] methods.

Sample	C (wt %)[a]	N (wt %)[a]	O (wt %)[a]	S (wt %)[a]	C (wt %)[b]	N (wt %)[b]	H (wt %)[b]
P*o*PD-30	72.53	18.68	8.27	0.52	69.17	18.78	3.88
P*o*PD-50	73.03	19.06	7.61	0.30	72.46	19.66	3.53
P*o*PD-70	73.11	19.57	7.00	0.32	72.98	20.34	3.15
P*o*PD-70-300	74.10	19.32	6.33	0.25	73.43	19.45	3.07

Table S2 Textural properties of P*o*PD-derived carbon materials.

Sample	S_{BET} (m^2 g^{-1})	V_{tot} (cm^3 g^{-1})	D (nm)
P*o*PD-C-400	12	0.026	9.5
P*o*PD-C-600	17	0.032	7.8
P*o*PD-C-800	93	0.083	3.6
P*o*PD-C-1000	240	0.147	2.5

S_{BET}: Specific surface area; V_{tot}: Total pore volume; D: Average pore diameter.

Table S3 The comparisons of catalytic performance between P*o*PD-derived materials and other reported metal-free catalysts.

Catalyst	Temperature (°C)	GHSV (h^{-1})	Conversion (%)	Reference
SiC@NC	200	30	80	S1
PDA/SiC-600	200	30	77	S2
ZIF-8/SAC	180	30	73	S3
Z_4M_1	180	50	60	S4
N,S-C-2.5	180	50	82	S5
N-CNTs	180	180	3.8	S6
N-MC-G	220	30	85.5	S7
PSAC-N0.8	250	120	68	S8
C_3N_4/AC	180	50	77	S9
N,P-C600	210	50	98.7	S10
N,S-C-NH_3	220	35	80	S11
C-NH_3(ZIF-8)	220	30	92	S12
AC-n-U500	240	30	92	S13
B,N-graphene	150	36	95	S14
NC1-1073	300	320	81	S15
3NR/4CAC	220	30	97.9	S16
PANI-AC	180	36	76	S17
N-OMC-O2.0	180	50	35	S18
N-MWCNTs	200	116	16.5	S19
ND@G	220	300	50	S20
C-1000	220	36	95	S21
D-AC-M	220	30	63	S22
MF-700	220	30	97	S23
p-BN	280	40	90	S24
P*o*PD-70-300	280	120	70	This work
P*o*PD-C-800	220	50	98.5	This work
P*o*PD-C-800	220	200	90.1	This work

Table S4 Compositions of C, N, and O (wt %) in P*o*PD-derived carbon materials determined by XPS.

Sample	C (wt %)	N (wt %)	O (wt %)
P*o*PD-C-400	72.06	13.18	14.76
P*o*PD-C-600	77.16	10.32	12.52
P*o*PD-C-800	79.11	8.53	12.36
P*o*PD-C-1000	81.93	5.91	12.16

Table S5 N species contents with binding energies in P*o*PD-derived carbon materials determined by XPS analysis.

Sample	N species contents with binding energies (at.%)			
	Pyridinic N	Pyrrolic N	Graphitic N	Pyridinic N-oxide
P*o*PD-C-400	45.56 (398.35 eV)	33.49 (399.68 eV)	18.69 (400.82 eV)	2.26 (402.64 eV)
P*o*PD-C-600	40.15 (398.37 eV)	22.80 (399.70 eV)	32.07 (400.70 eV)	4.98 (402.68 eV)
P*o*PD-C-800	38.27 (398.37 eV)	8.99(399.73 eV)	45.33 (400.93 eV)	7.41 (402.69 eV)
P*o*PD-C-1000	23.51 (398.32 eV)	6.55 (399.74 eV)	60.52 (400.98 eV)	9.42 (402.72 eV)

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