Supporting Information

Synergism between B-N atomic pair for promoting the catalytic cracking of 1,2-dichloroethane

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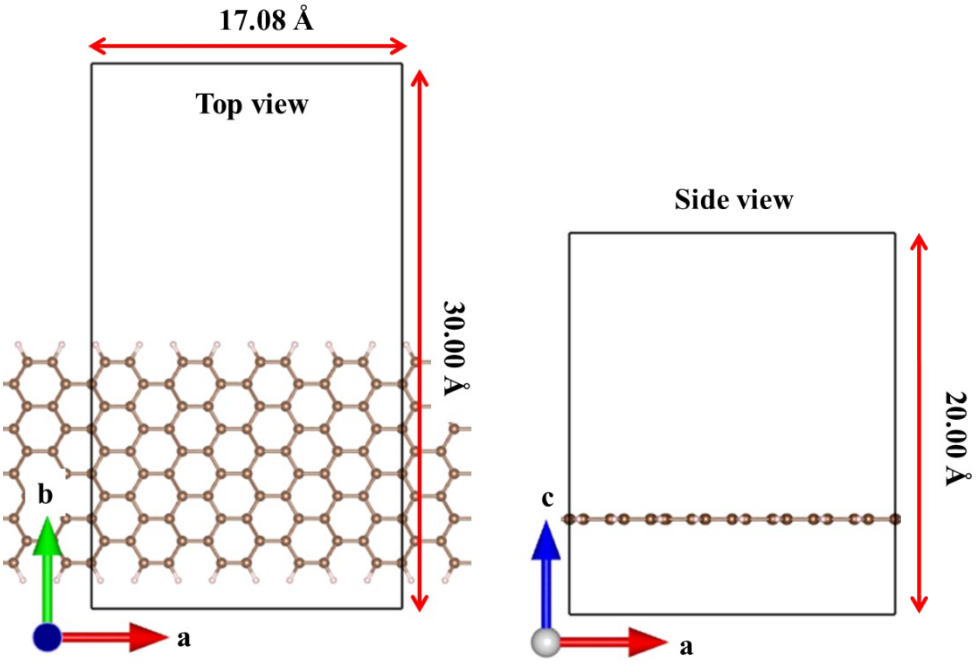

Figure S1 Structure of the hydrogen-terminated graphene nanoribbon with armchair edge.

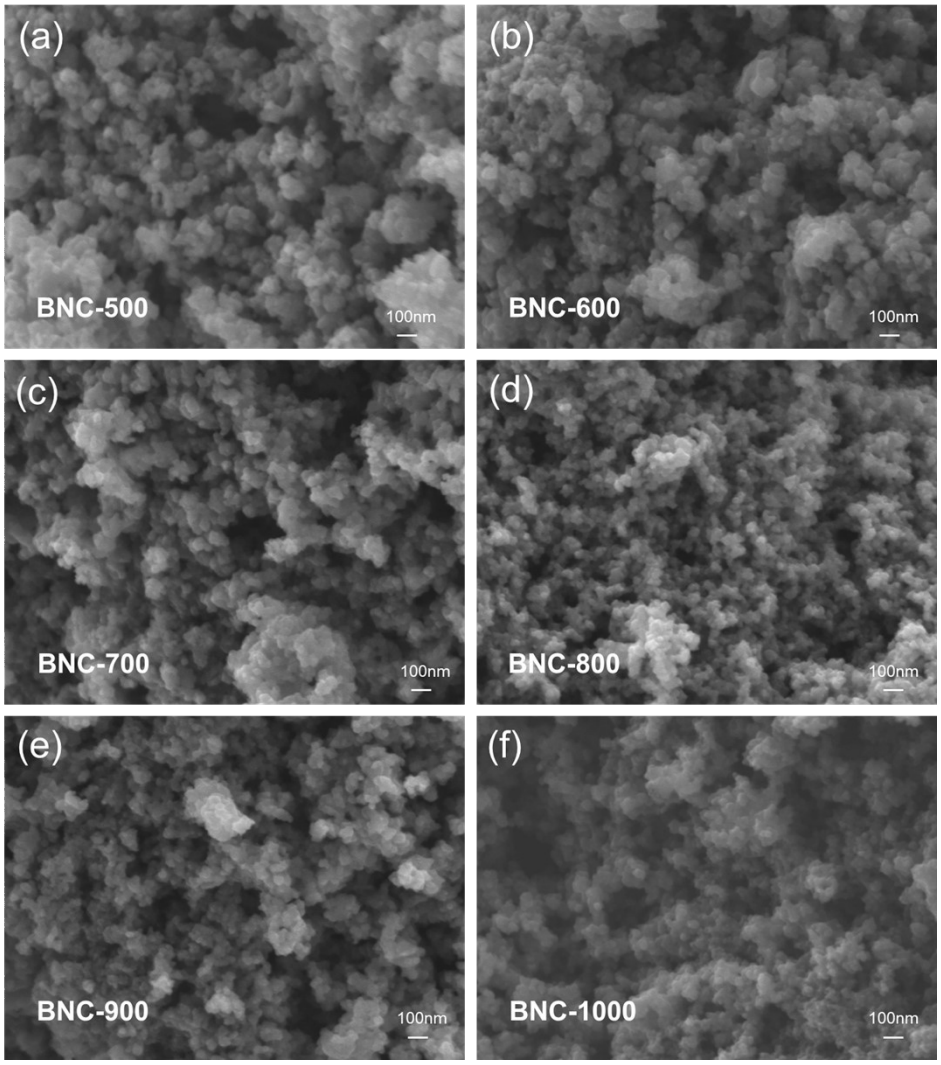

Figure S2 SEM images of (a) BNC-500, (b) BNC-600, (c) BNC-700, (d) BNC-800, (e) BNC-900, (f) BNC-1000.

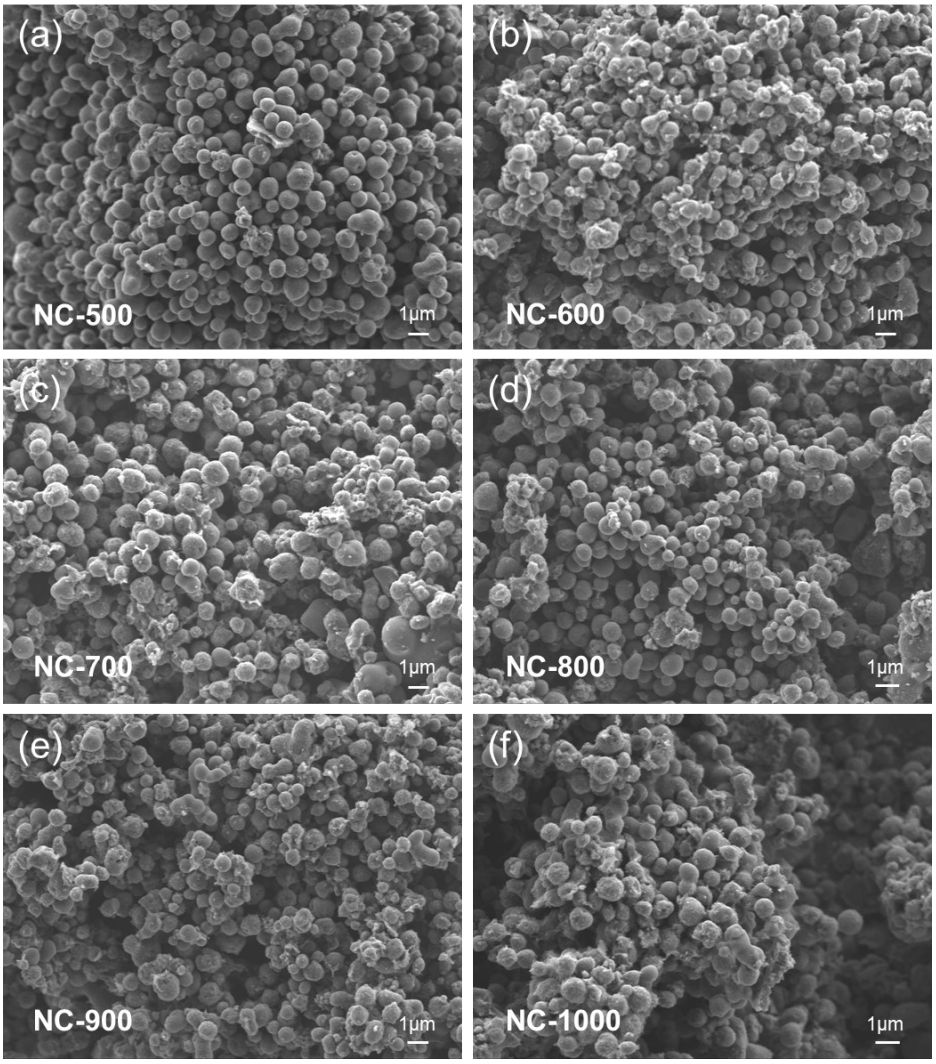

Figure S3 SEM images of (a) NC-500, (b) NC-600, (c) NC-700, (d) NC-800, (e) NC-900, (f) NC-1000.

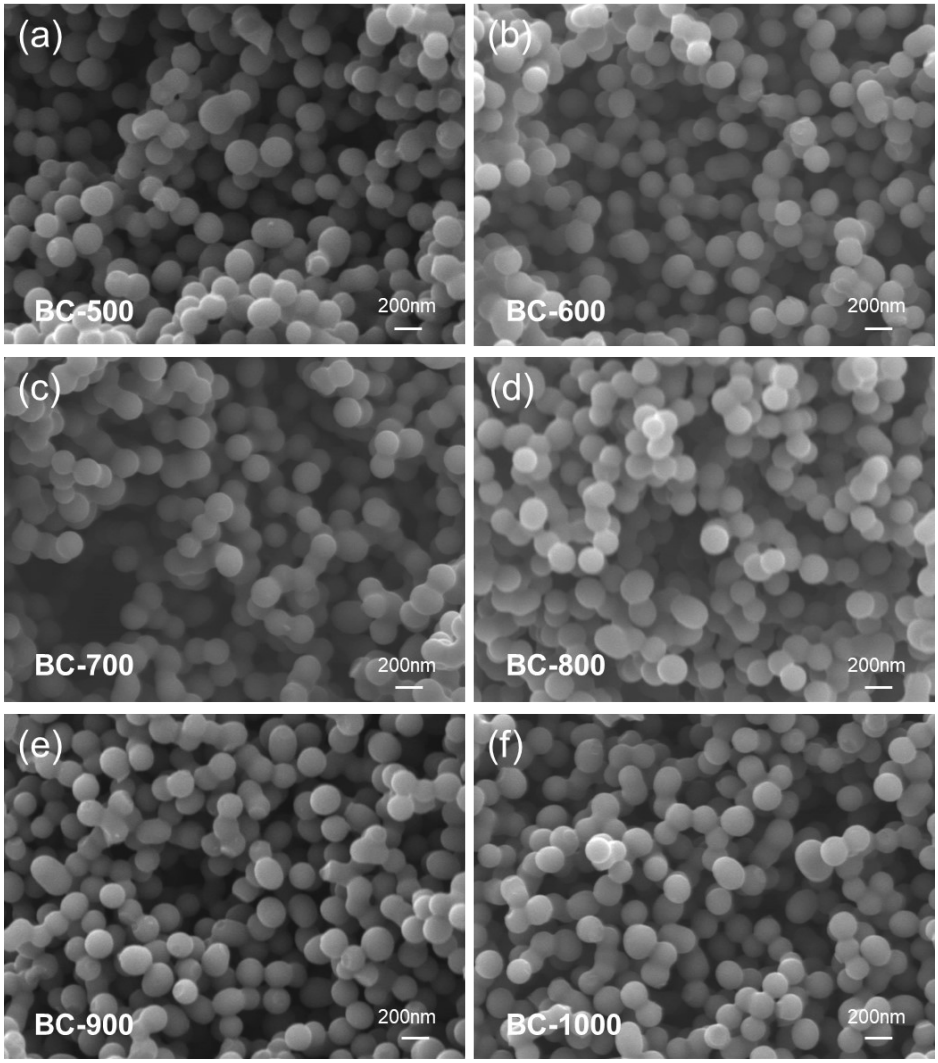

Figure S4 SEM images of (a) BC-500, (b) BC-600, (c) BC-700, (d) BC-800, (e) BC-900, (f) BC-1000.

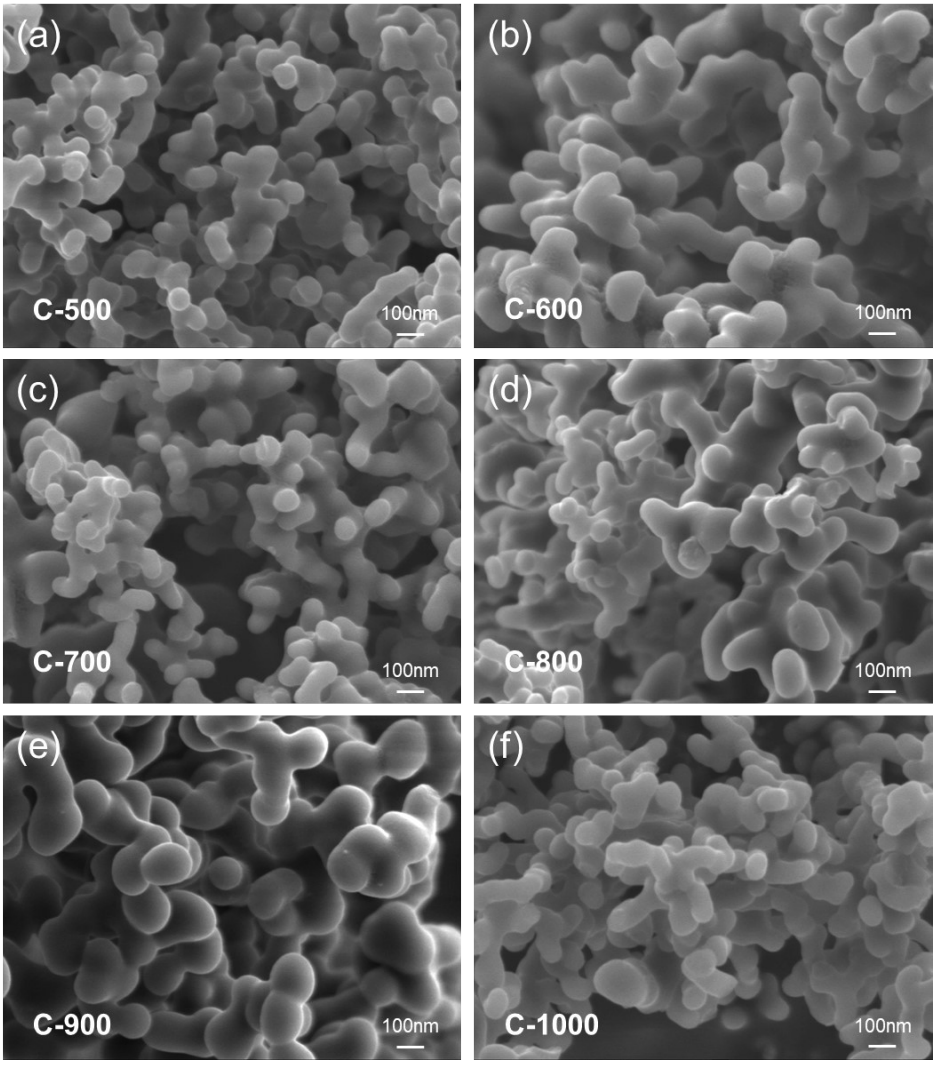

Figure S5 SEM images of (a) C-500, (b) C-600, (c) C-700, (d) C-800, (e) C-900, (f) C-1000.

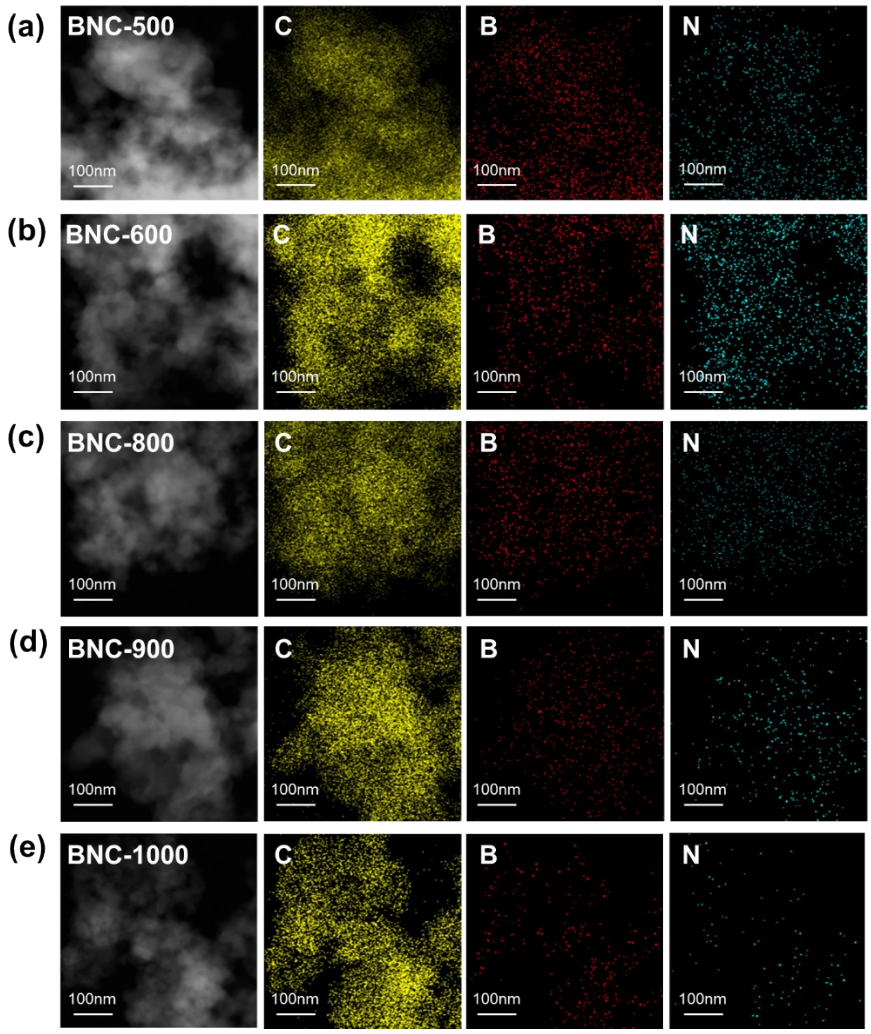

Figure S6 TEM images and elemental distribution mapping of C, B, N in (a) BNC-500, (b) BNC-600, (c) BNC-800, (d) BNC-900 and (e) BNC-1000.

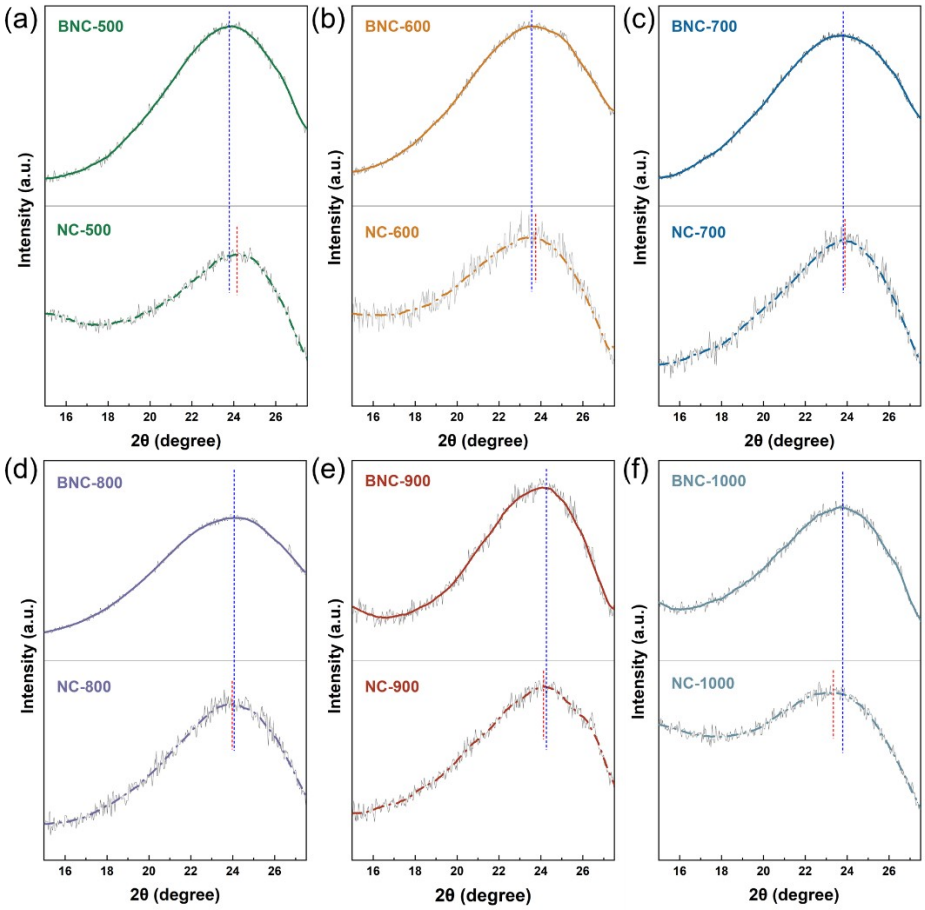

Figure S7 XRD patterns and peak shift of (a) BNC-500, (b) BNC-600, (c) BNC-700, (d) BNC-800, (e) BNC-900 and (f) BNC-1000.

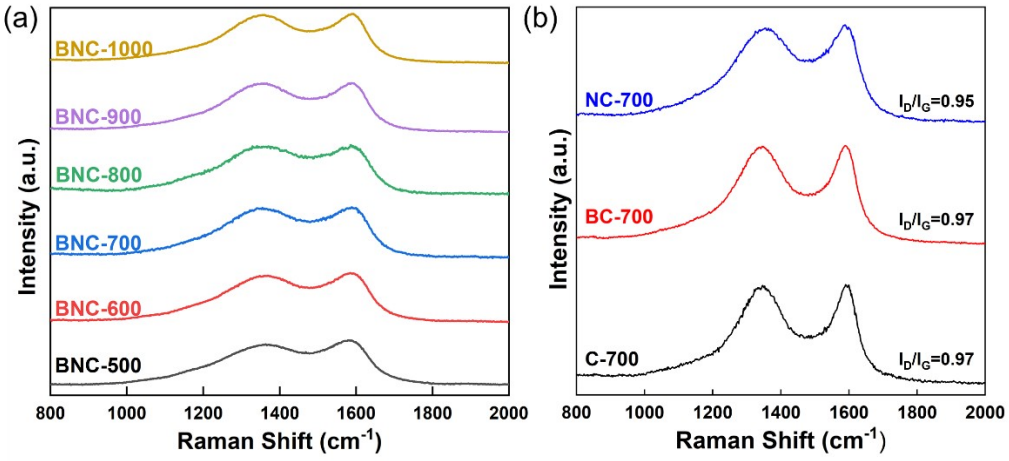

Figure S8 Raman spectra of (a) BNC with different calcination temperature and (b) NC, BC, C calcinated at 700 ℃

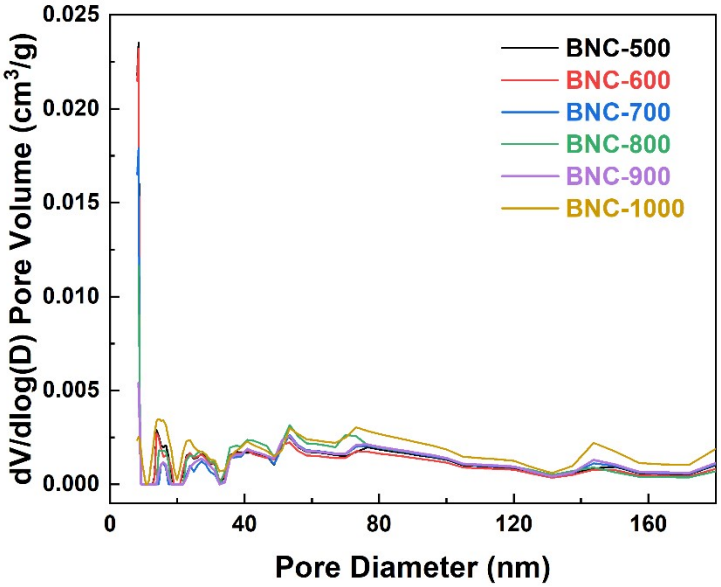

Figure S9 Pore size distribution of BNC

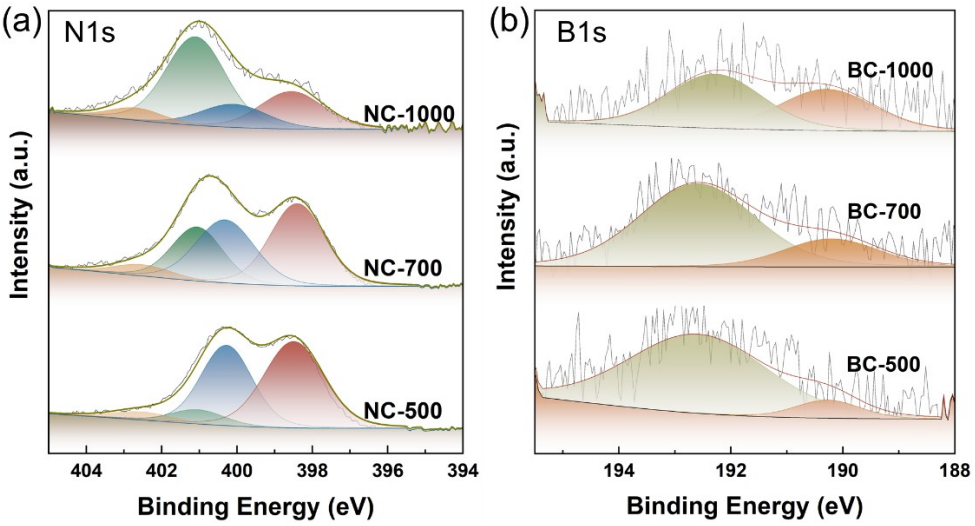

Figure S10 (a) XPS of N1s of NC; (b) XPS of B1s of BC.

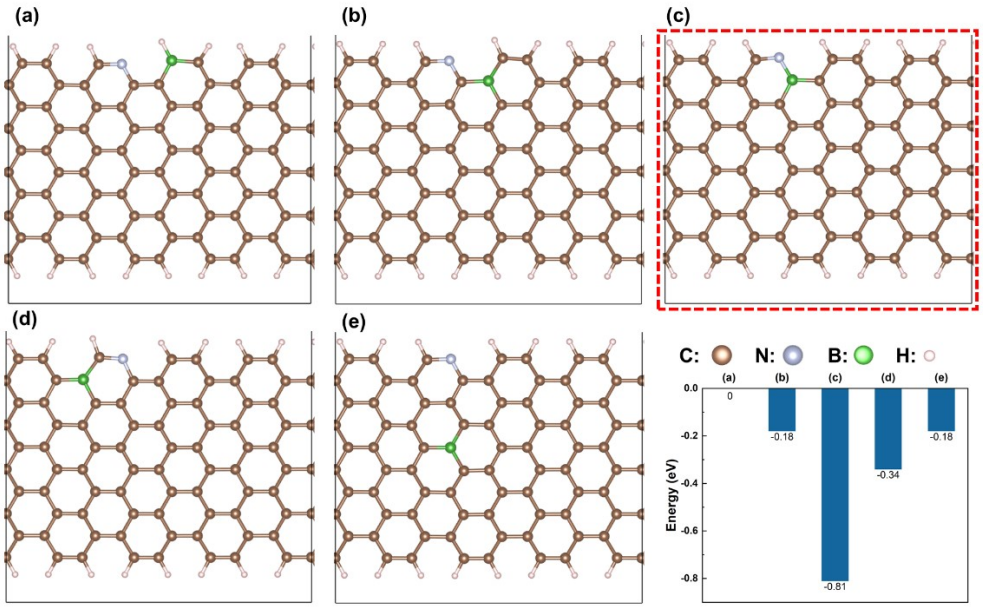

Figure S11 Different doping sites of B and their energy difference corresponding to a.

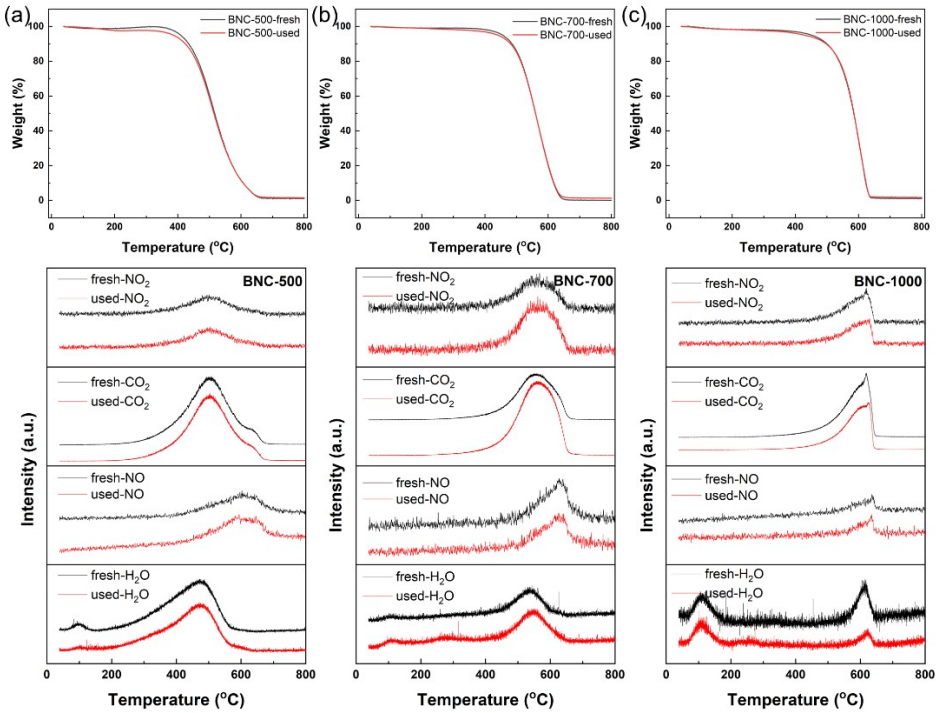

Figure S12 Thermogravimetric analysis curves recorded in air atmosphere and the removal of C, O and N in (a) BNC-500, (b) BNC-700 and (c) BNC-1000 catalysts before and after reaction

Table S1 The effect of the testing parameters on the energy.

ENCUT (eV)	$E_{gas+cat}$ (eV)	E_{Cat} (eV)	$E_{gas+cat}$ (eV)	*DE* (eV)
350	-832.4023028	-794.5408574	-37.70712987	-0.15431551
400	-831.5463520	-793.6631224	-37.70712987	-0.17609973
450	-831.1237741	-793.2398526	-37.70712987	-0.17679165
500	-831.0193745	-793.1388791	-37.70712987	-0.17336549

Table S2 The convergence test data of the vacuum layer

Vacuum layer (Å)	$E_{gas+cat}$ (eV)
15	-831.55424365
20	-831.54635200
25	-831.54279351

Table S3 The K-Point convergence test data

KPOINT	$E_{gas+cat}$ (eV)
1X1X1	-831.18945286
2X1X1	-831.54635200
3X3X3	-831.54279351

Table S4 Physical structure of C catalyst.

Sample	S_{BET} (m^2/g)	V_{pore} (cm^3/g)	V_{meso} (cm^3/g)
C-500	307	0.17	0.046
C-600	308	0.19	0.035
C-700	325	0.21	0.042
C-800	314	0.18	0.015
C-900	217	0.14	0.059
C-1000	17	0.023	0.022

Table S5 Physical structure of BC catalyst.

Sample	S_{BET} (m^2/g)	V_{pore} (cm^3/g)	V_{meso} (cm^3/g)
BC-500	346	0.22	0.033
BC-600	336	0.20	0.021
BC-700	352	0.22	0.029
BC-800	381	0.24	0.027
BC-900	246	0.16	0.058
BC-1000	286	0.14	0.17

Table S6 Physical structure of NC catalyst.

Sample	S_{BET} (m^2/g)	V_{pore} (cm^3/g)	V_{meso} (cm^3/g)
NC-500	103	0.15	0.11
NC-600	120	0.16	0.13
NC-700	111	0.14	0.10
NC-800	127	0.17	0.12
NC-900	118	0.21	0.17
NC-1000	115	0.20	0.15

Table S7 EDC conversion of NC, BC, C catalyst with different calcination temperature.

Sample \ T (°C)	500	600	700	800	900	1000
NC	16.3	14.4	10.2	8.37	6.69	5.05
BC	0.225	0.369	0.336	0.277	0.231	0.233
C	0.327	0.388	0.420	0.368	0.330	0.185

Table S8 The content of different N species in BNC catalyst before and after reaction.

Sample	Pyridinic N	Pyrrolic N	Graphitic N	Oxide N	B-N
BNC-500	35.15	43.66	7.75	7.35	6.09
BNC-500-used	29.46	41.28	18.15	6.51	4.60
BNC-700	25.65	28.14	23.06	7.80	15.36
BNC-700-used	22.72	30.21	37.27	4.82	4.99
BNC-1000	14.02	12.52	53.33	9.06	11.08
BNC-1000-used	8.59	16.15	63.44	6.26	5.56

Table S9 The content of different N species in NC catalyst

Sample	Pyridinic N	Pyrrolic N	Graphitic N	Oxide N
NC-500	48.92	39.17	7.28	4.63
NC-700	38.63	31.97	23.69	5.71
NC-1000	24.08	15.68	53.47	6.77

Table S10 Physical structure of BNC catalyst after reaction.

Sample	S_{BET} (m^2/g)	V_{pore} (cm^3/g)	V_{meso} (cm^3/g)
BNC-500-used	83	0.30	0.28
BNC-600-used	85	0.31	0.29
BNC-700-used	80	0.46	0.45
BNC-800-used	69	0.38	0.38
BNC-900-used	74	0.35	0.34
BNC-1000-used	73	0.36	0.35