Supplementary Information

Synergy of nitrogen vacancies and partially broken hydrogen bonds in graphitic carbon nitride for superior photocatalytic hydrogen evolution under visible light

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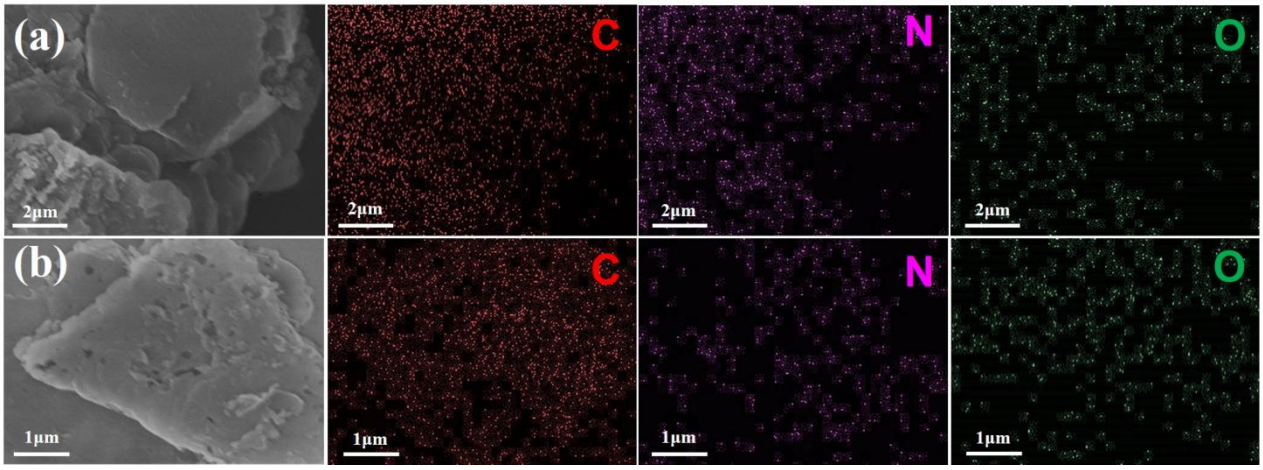

Fig. S1 SEM and elements mapping images of (a) HCN and (b) BCN.

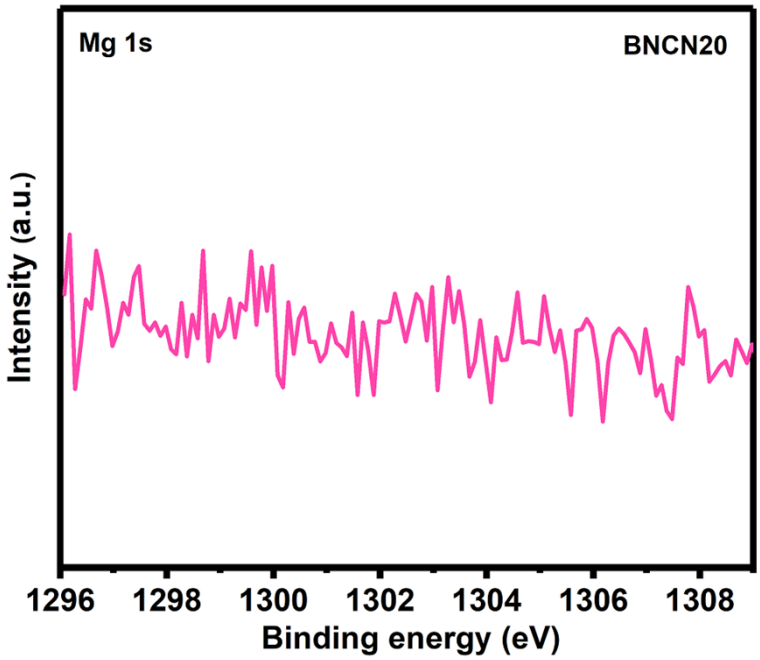

Fig. S2 Mg 1s XPS of BNCN20 sample.

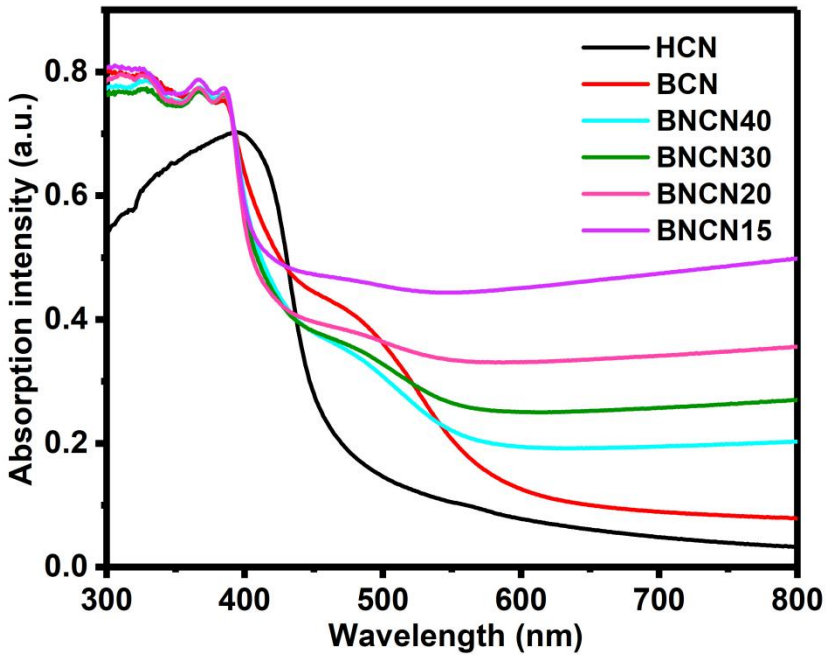

Fig. S3 UV-visible absorption spectroscopy of HCN, BCN and BNCNx with different weight ratios (40~15).

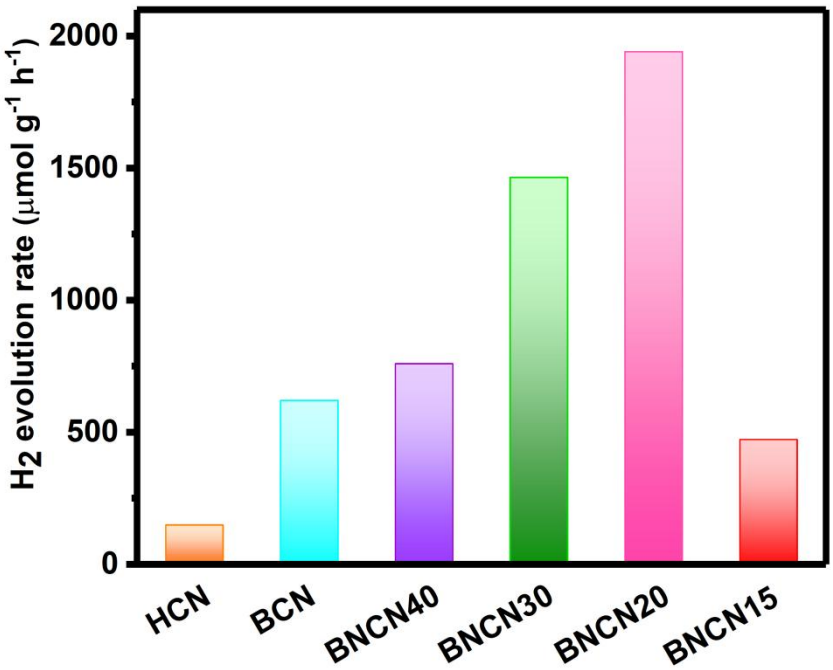

Fig. S4 Photocatalytic hydrogen production of HCN, BCN and BNCNx with different weight ratios (40~15) under visible-light irradiation (λ > 400 nm).

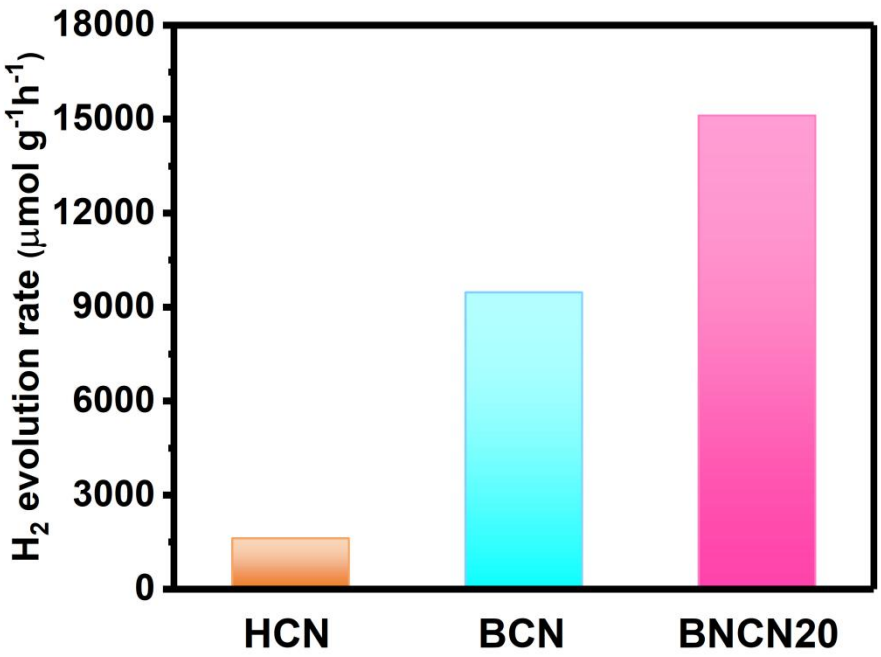

Fig. S5 Photocatalytic hydrogen evolution performances of as-prepared HCN, BCN and BNCN20 with 1.5 wt% Pt under white light illumination.

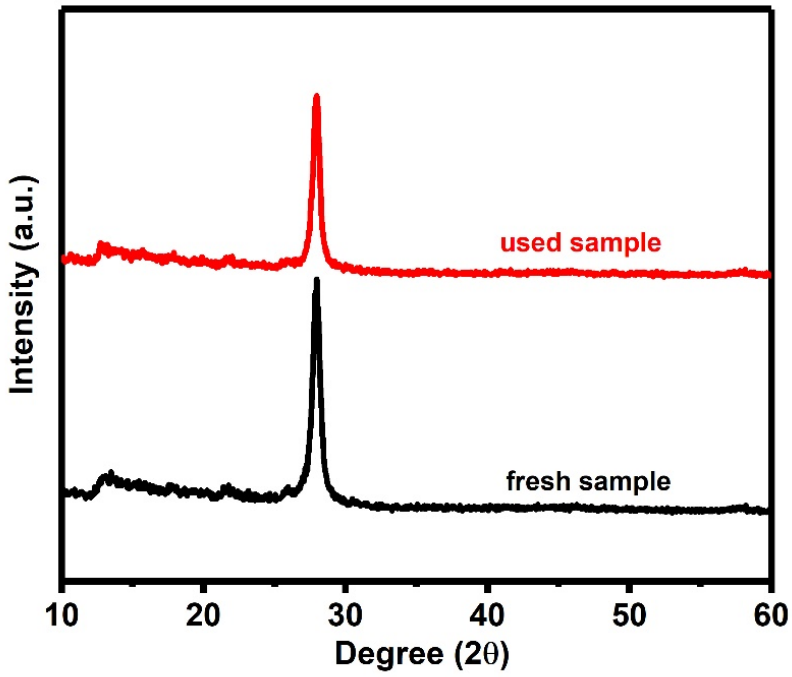

Fig. S6 XRD patterns of the BNCN20 before and after four circulating runs of hydrogen production.

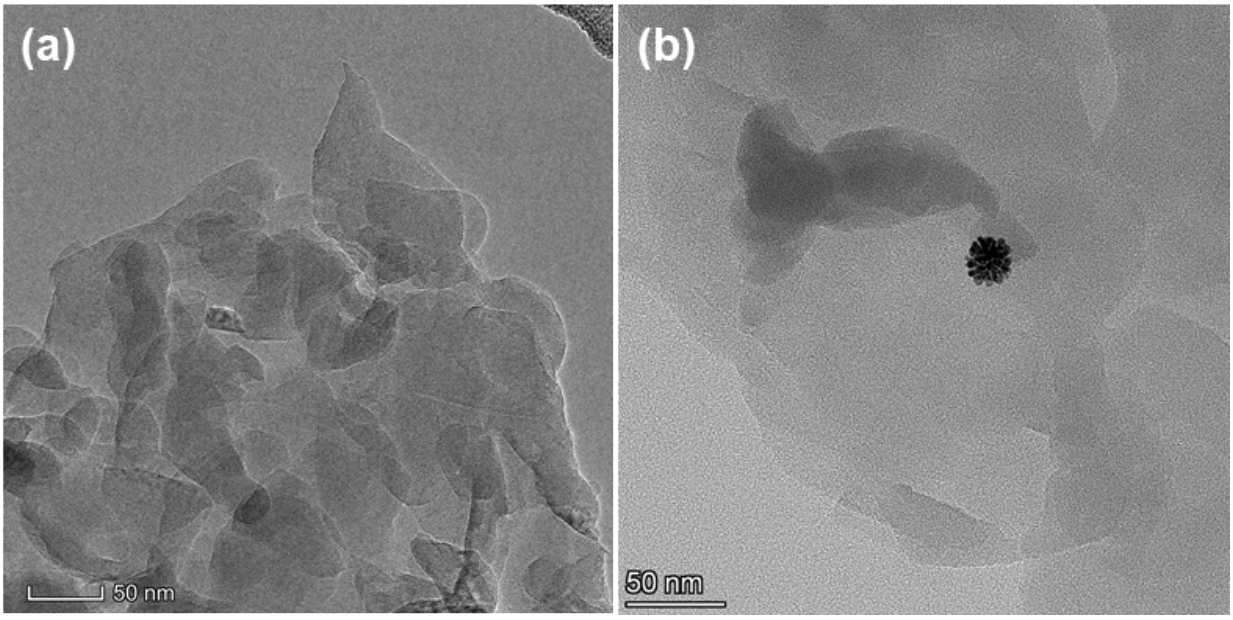

Fig. S7 TEM image of the BNCN20 after four circulating runs of hydrogen production.

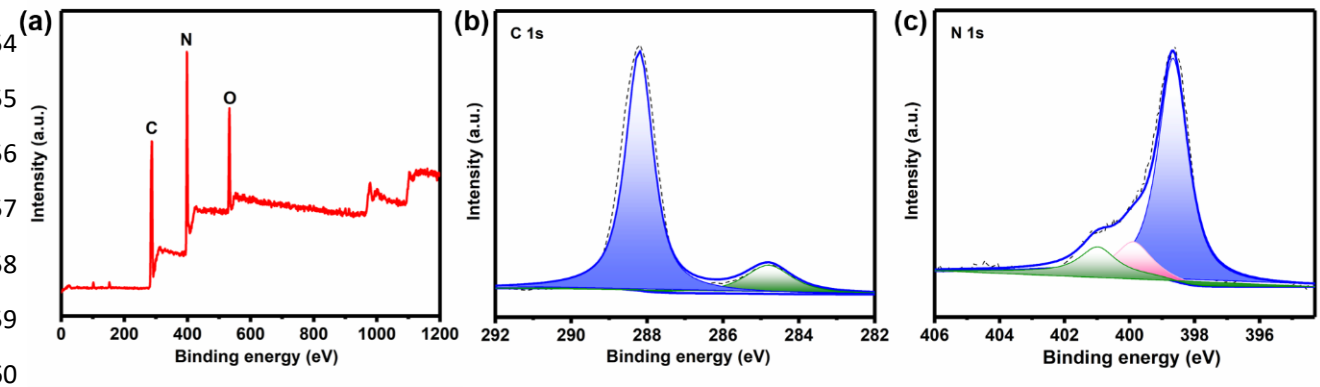

Fig. S8 XPS spectra of the used BNCN20: (a) Survey, (b) N1s, and (c) N1s.

Table S1. Summarized N_2 adsorption-desorption isotherm data for HCN, BCN, and BNCN.

Sample	S_{BET} [m^2 g^{-1}]	S_{ext}[1] [m^2 g^{-1}]	S_{micro} [m^2 g^{-1}]	V_{tol}[2] [cm^3 g^{-1}]	V_{micro} [cm^3 g^{-1}]	V_{meso}[3] [cm^3 g^{-1}]
HCN	3.2342	4.3566	—	0.06054	—	0.06054
BCN	28.6470	20.8378	7.8092	0.195879	0.003322	0.192557
BNCN20	40.3037	36.0487	4.2549	0.2564	0.001959	0.254402

1 Determined from t-plot method.

2 Determined from adsorbed volume at $P/P_0 = 0.98$.

3 $V_{meso}=V_{tol}-V_{micro}$.

Table S2. The deconvolution results of C 1s and N 1s XPS spectra of HCN, BCN, and BNCN20.

	C (eV)		N (eV)				
Samples	N-C=N	C-C/C=C	NH_x	N_{3C}	N_{2C}	NH_x/N_{3C}	N_{2C}/N_{3C}
HCN	288.2	284.8	401.0	400.1	398.5	0.88	7.89
BCN	288.2	284.8	401.0	400.1	398.5	0.77	7.85
BNCN20	288.2	284.8	401.0	399.8	398.5	0.68	5.98

Table S3. Relative quantification of the Solid-State MAS 13C NMR spectra of HCN, BCN and BNCN20 samples.

Sample	C3/C2
HCN	1.49
BCN	1.42
BNCN20	1.92

Table S4. The apparent quantum efficiency of HCN, BCN and BNCN20 (loaded with 1.5wt% Pt by in-situ photoreduction) under different wavelengths.

AQE / Sample	405 nm	420 nm	435 nm	450 nm	475 nm	500 nm
HCN	0.68%	0.40%	0.12%	0	0	0
BCN	2.12%	2.29%	3.19%	2.84%	0	0
BNCN20	9.58%	8.57%	8.38%	4.21%	2.91%	0

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