## Polymeric carbon nitride with frustrated Lewis pair sites for enhanced photofixation of nitrogen

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Figure S1. Elemental mapping of B, C and N elements in 10B-C<sub>3</sub>N<sub>4</sub>.



Figure S2. FT-IR spectra (a) and the enlarged view (b) of  $C_3N_4$ , 10Mo- $C_3N_4$ , 10B-C N = 10P/10Ma C N

 $C_3N_4$ , 10B/10Mo- $C_3N_4$ .



Figure S3. XPS S2p spectrum of 10B/10Mo-C<sub>3</sub>N<sub>4</sub>.

Table S1. The atomic content for C, N, B, Mo, O elements in C<sub>3</sub>N<sub>4</sub> and 10B/10Mo-

$C_3N_4$ from XP	'S characterization.
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	С	Ν	В	Mo	0
$C_3N_4$	38.19	57.53	-	-	4.28
10B/10Mo-C <sub>3</sub> N <sub>4</sub>	36.62	57.48	0.22	0.62	5.06



Figure S4. The time-dependent absorbance increasement at 420 nm over  $C_3N_4$ , xMo- $C_3N_4$ , xB- $C_3N_4$  and xB/xMo- $C_3N_4$ .

**Table S2.** Yield of the products via reaction over 10B/10Mo-C<sub>3</sub>N<sub>4</sub> photocatalysts under different condition.

Entr	Catalyst	Atmospher	Irradiatio	NH <sub>3</sub>	$\mathrm{H}_{2}$	$N_2H_4$
У		e	n	productio	productio	productio
				n rate	n rate	n rate
1	10B/10Mo	$N_2$	Light	1.68	0.05	Not
	-C <sub>3</sub> N <sub>4</sub>					detected
2	10B/10Mo	Ar	Light	Not		
	-C <sub>3</sub> N <sub>4</sub>			detected		
3	10B/10Mo	$N_2$	Dark	Not		
	-C <sub>3</sub> N <sub>4</sub>			detected		





2.0 I-H 1.5 0.5 H 0.0 1.5 0.5 Number of cycles

under monochromatic light irradiation.

Figure S6. Repeated cycles of photocatalytic NH<sub>3</sub> production of 10B/10Mo-



Figure S7. XRD pattern of 10B/10Mo-C<sub>3</sub>N<sub>4</sub> after cycling test.

Table S3. Average fluorescence lifetime of C<sub>3</sub>N<sub>4</sub>, 10Mo-C<sub>3</sub>N<sub>4</sub>, 10B-C<sub>3</sub>N<sub>4</sub> and

$10B/10Mo-C_3N_4.$		
	lifetime (ns)	
$C_3N_4$	12.54	
10B-C <sub>3</sub> N <sub>4</sub>	17.08	



Figure S8. EIS Nyquist plots of  $C_3N_4$ , 10Mo- $C_3N_4$ , 10B- $C_3N_4$ , 10B/10Mo- $C_3N_4$  in



Figure S9. EIS Nyquist plots of  $10B/10Mo-C_3N_4$  under Ar and  $N_2$  atmosphere with light illumination.



Figure S10. Transient photocurrents of  $10B/10Mo-C_3N_4$  under Ar and  $N_2$  atmosphere.



Figure S11. VB XPS spectra of  $C_3N_4$  (a) and  $10B-C_3N_4$  (b).