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Electronic supplementary information (ESI)

Boosted photocatalytic nitrogen fixation by bismuth and oxygen vacancies in Bi_2MoO_6/BiOBr composite structures

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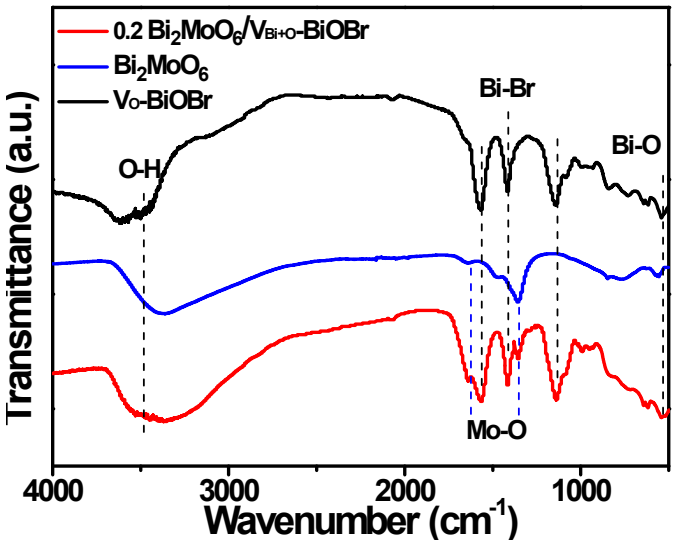

Fig. S1 FT-IR spectrum of Bi_2MoO_6, V_O-BiOBr and 0.2 Bi_2MoO_6/V_{Bi+O}-BiOBr samples, respectively.

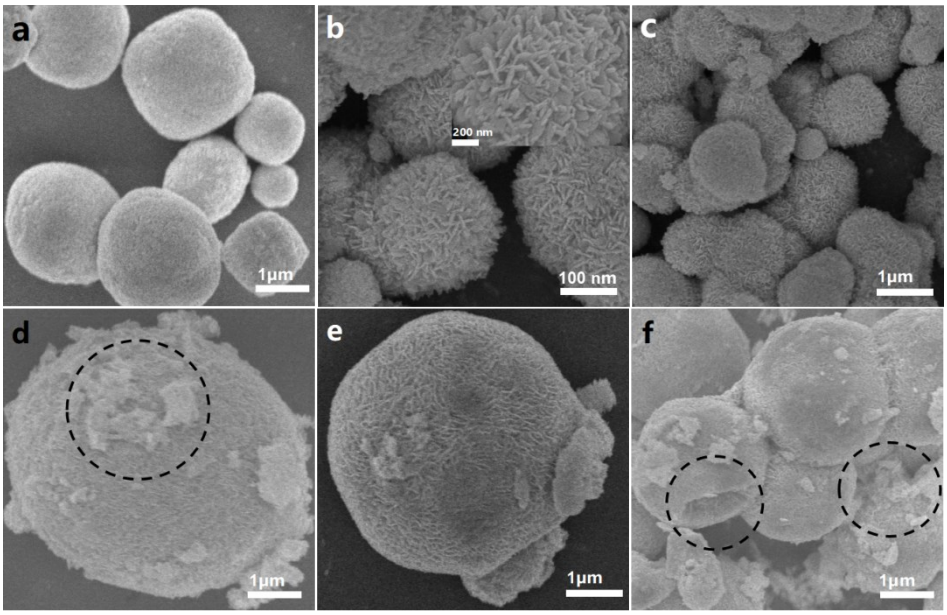

Fig. S2 (a) SEM images of Vo-BiOBr, (b-c) Bi_2MoO_6, (d-e) 0.1 Bi_2MoO_6/V_{Bi+O}-BiOBr and (f) 0.3 Bi_2MoO_6/V_{Bi+O}-BiOBr composite.

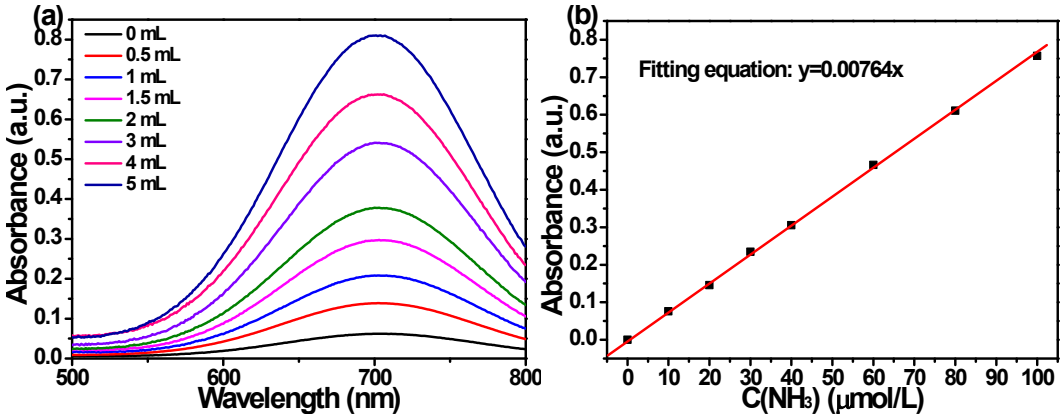

Fig. S3 Calibration for NH_4^+ determination. (a) Absorption spectra of ammonia chloride solutions with different concentrations through the indophenol blue method and (b) Linear relationship between the peak absorbance at 700 nm and the NH_4^+ concentration.

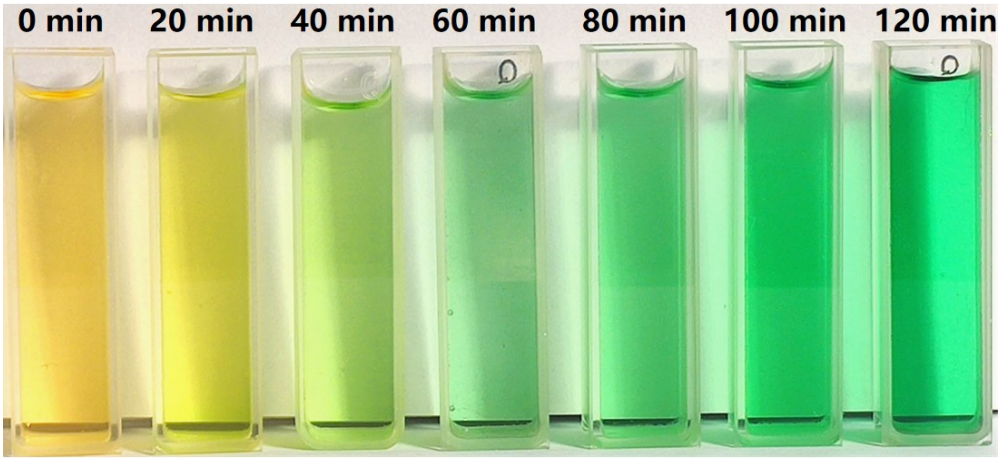

Fig. S4 Photograph of the aliquots obtained during N_2 photofixation with the 0.2 Bi_2MoO_6/V_{Bi+O}-BiOBr sample and subjected to the indophenol-blue test. The colors of the solutions change gradually with the irradiation time.

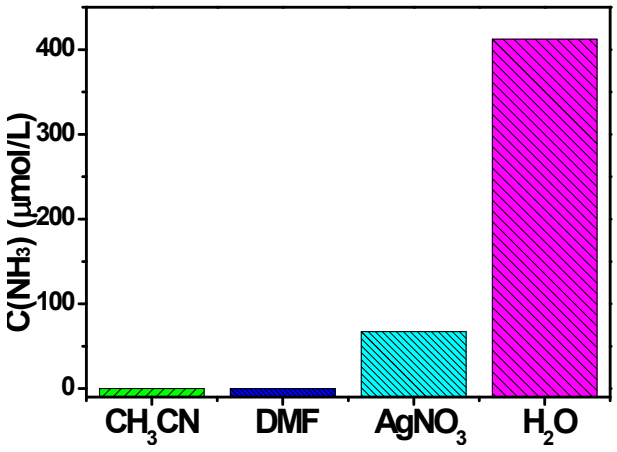

Fig. S5 Photocatalytic N_2 fixation with using aprotic solvents (CH_3CN and DMF) instead of water or added $AgNO_3$ as the electron scavenger.

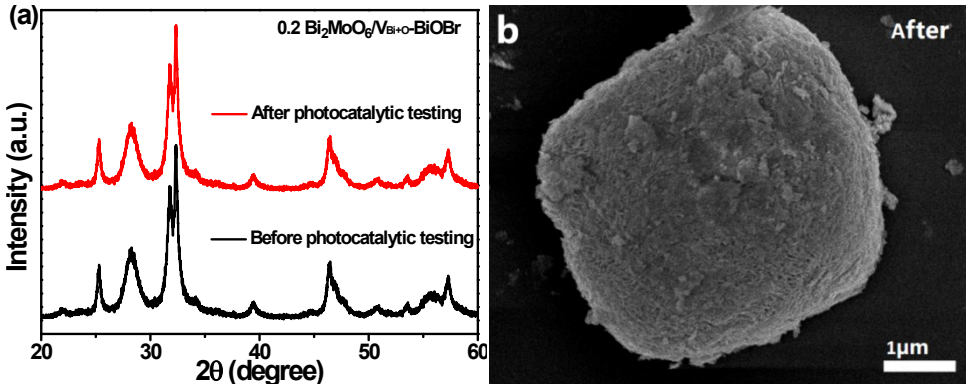

Fig. S6 (a) XRD patterns and (b) SEM image of 0.2 Bi_2MoO_6/V_{Bi+O}-BiOBr before and after five cycles of photocatalytic nitrogen fixation tests.

Table S1. XPS surface element analysis of the V_O-BiOBr and 0.2 Bi_2MoO_6/V_{Bi+O}-BiOBr samples.

Sample	Bi atom%	O atom%	Br atom%	Mo atom%	Bi :O
V_O-BiOBr	**24.38**	**31.25**	**24.82**	**0**	**0.78:1**
0.2 Bi_2MoO_6/V_{Bi+O}-BiOBr	**21.52**	**29.83**	**23.16**	**4.15**	**0.72:1**

Table S2. Elemental composition of the V_O-BiOBr and 0.2 Bi_2MoO_6/V_{Bi+O}-BiOBr samples by inductively coupled plasma mass spectrometry (ICP-MS).

Sample	Bi atom%	O atom%	Br atom%	Mo atom%	Bi :O
V_O-BiOBr	**25.64**	**30.16**	**28.94**	**0**	**0.85:1**
0.2 Bi_2MoO_6/V_{Bi+O}-BiOBr	**24.77**	**30.98**	**29.15**	**4.24**	**0.80:1**

Table S3. Comparison of the photocatalytic performance of relevant catalysts towards N_2 fixation.

Catalyst	Reaction medium	Scavenger	Light source	Ammoniageneration rate	Reference
0.2 Bi_2MoO_6/V_{Bi+O}-BiOBr	H_2O(l), 25 ℃	No	300 W Xe lamp, Full range light	206 μmol/L/h	This work
V_O-BiOBr nanosheets	H_2O(l), 25 ℃	No	300 W Xe lamp, Full range light	54.7 μmol/g/h	S10
BiOBr-001-OV	H_2O(l), 25 ℃	No	300 W Xe lamp, λ > 420 nm	104.2 μmol/g/h	S11
5 nm Bi_5O_7Br-NT	H_2O(l), 25 ℃	No	300 W Xe lamp, λ > 400 nm	1.38 mmol/g/h	S39
defect-rich SUC Bi_3O_4Br	H_2O(l), 25 ℃	No	300 W Xe lamp, λ > 400 nm	25.4 μmol/L/h	S15
p-n Bi_2MoO_6/ OV-BiOBr	H_2O(l), 25 ℃	No	300 W Xe lamp, λ > 400 nm	90.7 μmol/g//h	S21
0.5% Fe-Bi_2MoO_6	H_2O(l), 25 ℃	No	300 W Xe lamp, λ > 400 nm	106.5 μmol/g/h	S25
Bi_5O_7Br-40℃	H_2O(l), 25 ℃	No	300 W xenon lamp (200-800 nm)	12.72 mmol/g/h	S32
BiOBr-Fe-S-1	H_2O(l), 25 ℃	No	300 W Xe lamp, λ > 400 nm	46.1 μmol/g/h	S12