

Interfacial synergy of Pt cocatalyst and oxygen defective Bi₂MoO₆ for boosting photocatalytic redox reaction

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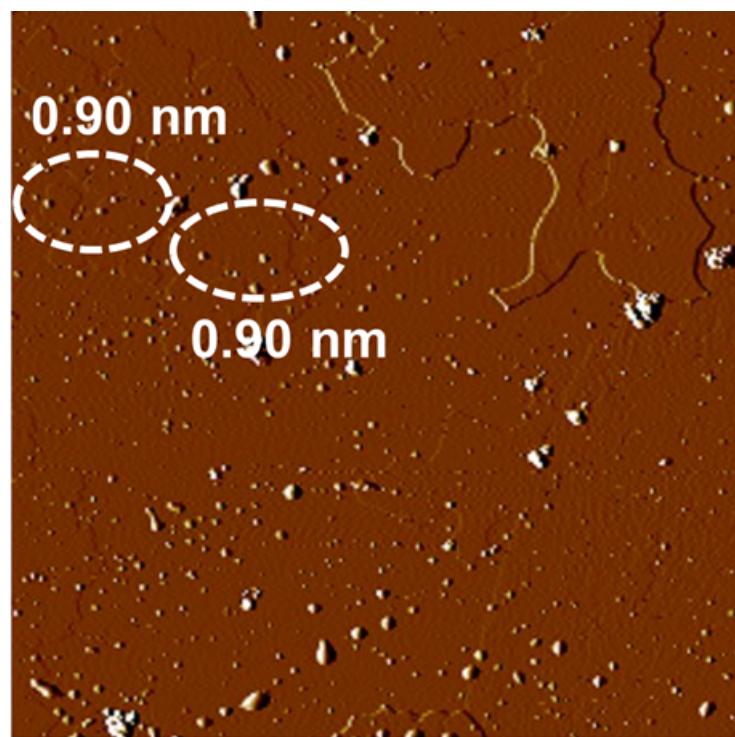


Fig. S1 AFM image of $\text{Bi}_2\text{MoO}_6\text{-V}_\text{O}$ catalyst

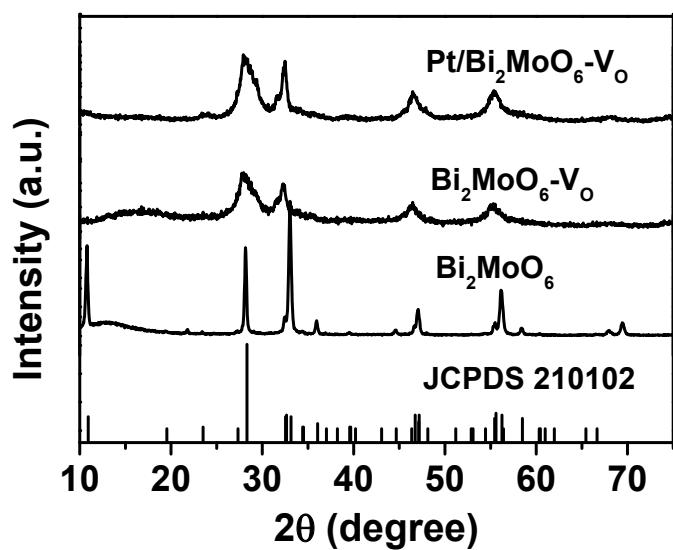


Fig. S2 XRD patterns of Bi_2MoO_6 samples

Table S1 The concentration of surface oxygen vacancies (V_O) and lattice oxygen (O_{latt}) for Bi_2MoO_6 catalysts

Catalysts	$V_O / (V_O + O_{latt})$	$O_{latt} / (O_{latt} + V_O)$
Bi_2MoO_6	0.15	0.85
$Bi_2MoO_6-V_O$	0.20	0.80
Pt/ $Bi_2MoO_6-V_O$	0.37	0.63

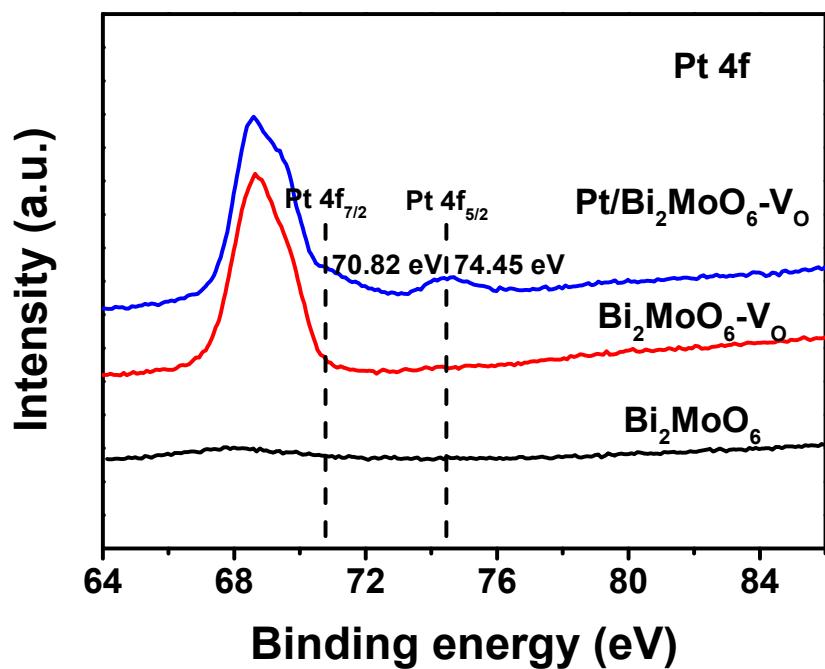


Fig. S3 Pt 4f XPS spectra of Bi₂MoO₆ samples

Table S2 Black experiments

Entry	Light	Photocatalyst	O ₂	Conversion rate (%)	Selectivity (%)
1	+	+	+	41	99
2	-	+	+	<1	-
3	+	-	+	<1	-
4	+	+	-	<1	-

Reaction conditions: Pt/Bi₂MoO₆-V_O catalyst, 10 mg; benzyl alcohol, 0.1 mmol; C₆H₅CF₃, 1.5 mL; reaction time, 1 h; O₂, 0.1 MPa.

Table S3 The photoactivity of Bi_2MoO_6 photocatalyst reported in the literature so far

Reference	Catalyst	Catalyst mass (mg)	Conversion rate (%)	Time (h)	Photoactivity (mmol g ⁻¹ h ⁻¹) ¹⁾	Selectivity (%)
1	Pt/ Bi_2MoO_6 -glycerol	10	36	1	3.6	99
2	Bi_2MoO_6 spheres	16	38	4	0.6	99
3	Pd(0.05)/BMO-SOVs	20	58	3	0.97	99
This work	Pt/ Bi_2MoO_6 -V _O	10	41	1	4.1	99

References:

1. B. Zhang, J. Li, Y. Y. Gao, R. F. Chong, Z. L. Wang, L. Guo, X. W. Zhang, C. Li, To boost photocatalytic activity in selective oxidation of alcohols on ultrathin Bi_2MoO_6 nanoplates with Pt nanoparticles as cocatalyst, *J. Catal.*, 2017, **345**, 96-103.
2. K. Q. Jing, W. Ma, Y. H. Ren, J. H. Xiong, B. B. Guo, Y. J. Song, S. J. Liang, L. Wu, Hierarchical Bi_2MoO_6 spheres in situ assembled by monolayer nanosheets toward photocatalytic selective oxidation of benzyl alcohol, *Appl. Catal., B*, 2019, **243**, 10-18.
3. Z. L. Sun, X. L. Yang, X.-F. Yu, L. H. Xia, Y. H. Peng, Z. Li, Y. Zhang, J. B. Cheng, K. S. Zhang, J. Q. Yu, Surface oxygen vacancies of Pd/ $\text{Bi}_2\text{MoO}_{6-x}$ acts as "Electron Bridge" to promote photocatalytic selective oxidation of alcohol, *Appl. Catal., B*, 2021, **285**, 119790.

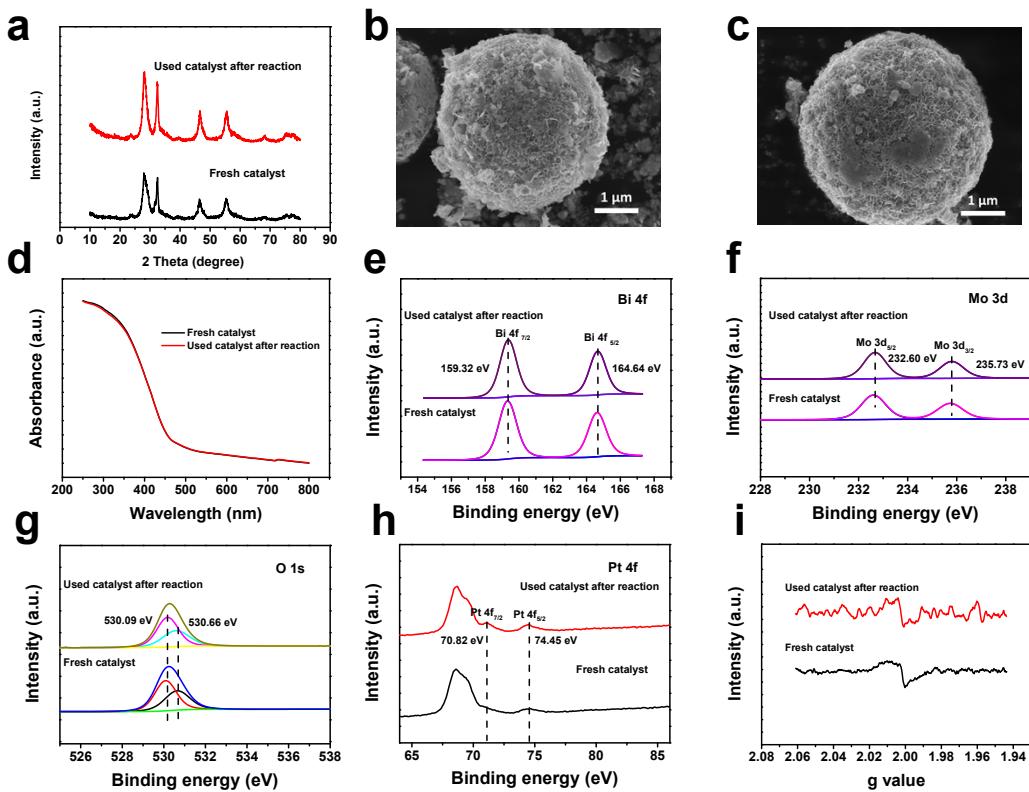


Fig. S4 Characterizations of Pt/Bi₂MoO₆-V_O catalysts before and after the reaction. (a) XRD patterns of Pt/Bi₂MoO₆-V_O samples before and after reaction. (b-c) SEM images of Pt/Bi₂MoO₆-V_O samples before and after reaction. (d) UV-Visible spectra of Pt/Bi₂MoO₆-V_O samples before and after reaction. (e-h) Bi 4f, Mo 3d, O1s, and Pt 4f XPS spectra of Pt/Bi₂MoO₆-V_O samples before and after reaction. (i) EPR spectra of Pt/Bi₂MoO₆-V_O samples before and after reaction.

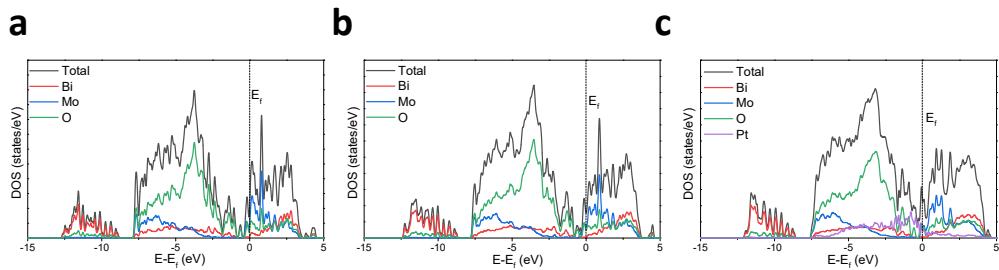


Fig. S5 Total and projected density of states (PDOS) of (a) Bi_2MoO_6 (001) surface, (b) Bi_2MoO_6 (001) surface with one oxygen vacancy, (c) Bi_2MoO_6 (001) surface with one oxygen vacancy and Pt_{13} loading. The dashed lines represent that the Fermi level is set to 0 eV.