Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers.

Band gap engineering of porous $BiVO_4$ nanoshuttles by Fe and Mo co-doping for efficient photocatalytic water oxidation

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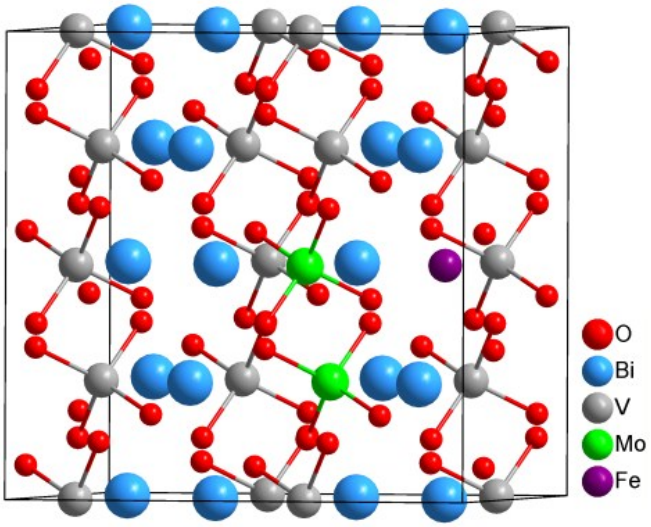


Fig. S1 The supercell model of Fe, Mo-BVO PNSs considered in this work.

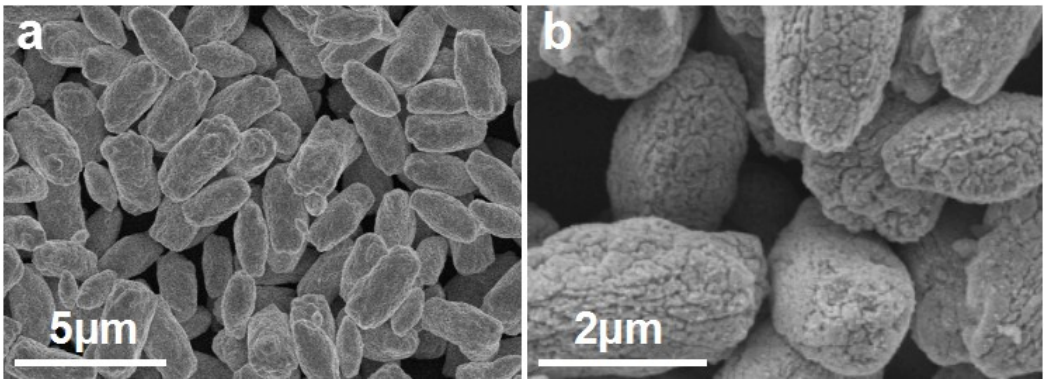


Fig. S2 SEM images of the as-prepared Fe-BVO samples.

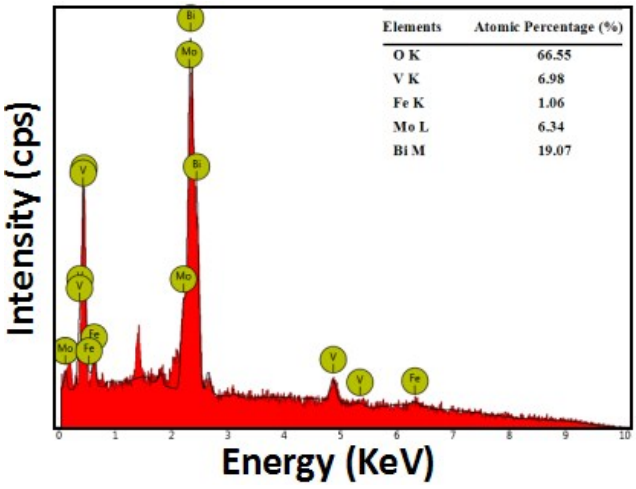


Fig. S3 EDS pattern of the as-prepared Fe/Mo-BVO PNSs and the atom percentages of O, V, Fe, MO and Bi elements (inset).

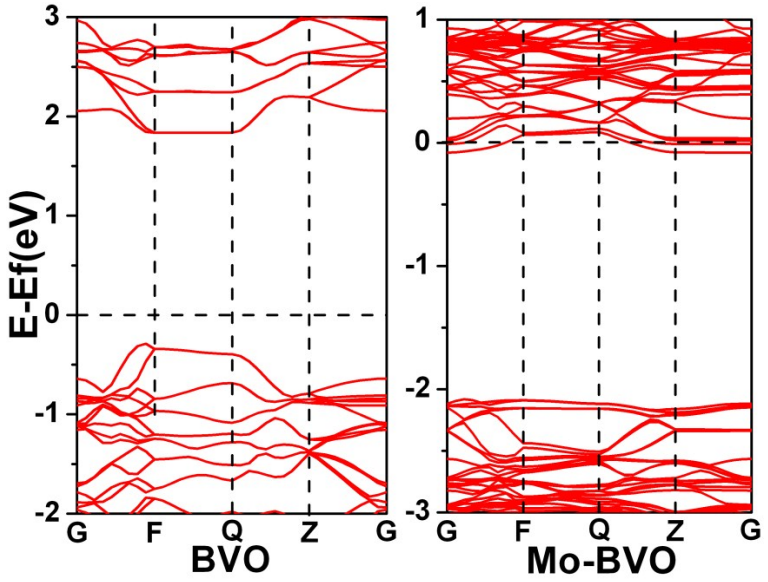


Fig. S4 The band structures calculated for the BVO and Mo-BVO crystal structures.

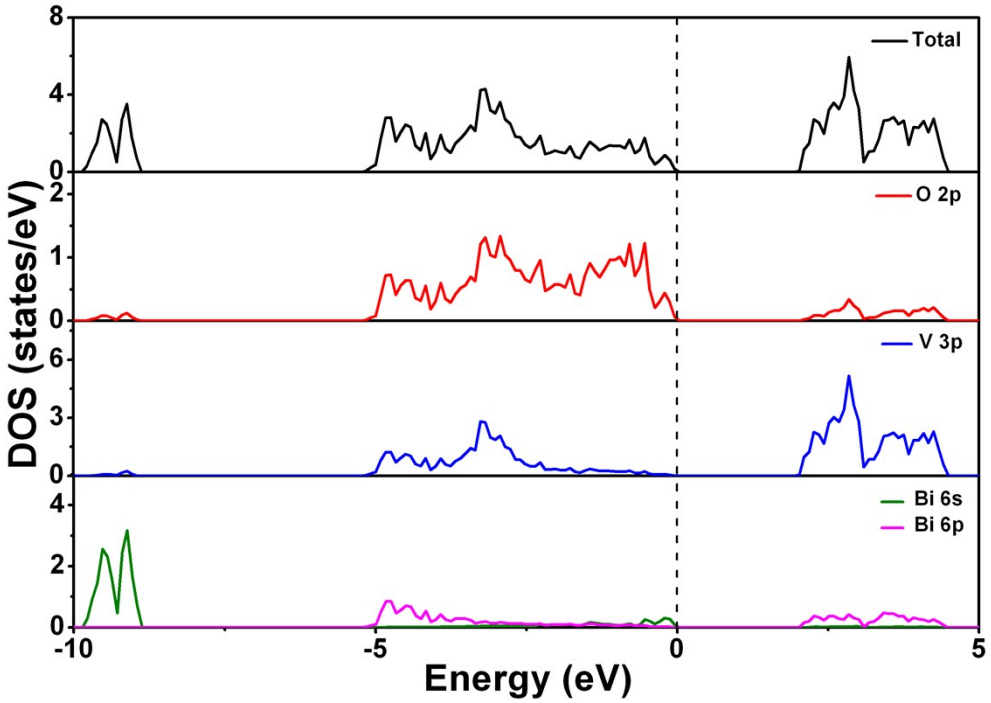


Fig. S5 Total DOS and the corresponding PDOSs of O2p, V3p, Bi 6s and Bi 6p states of pure BVO.

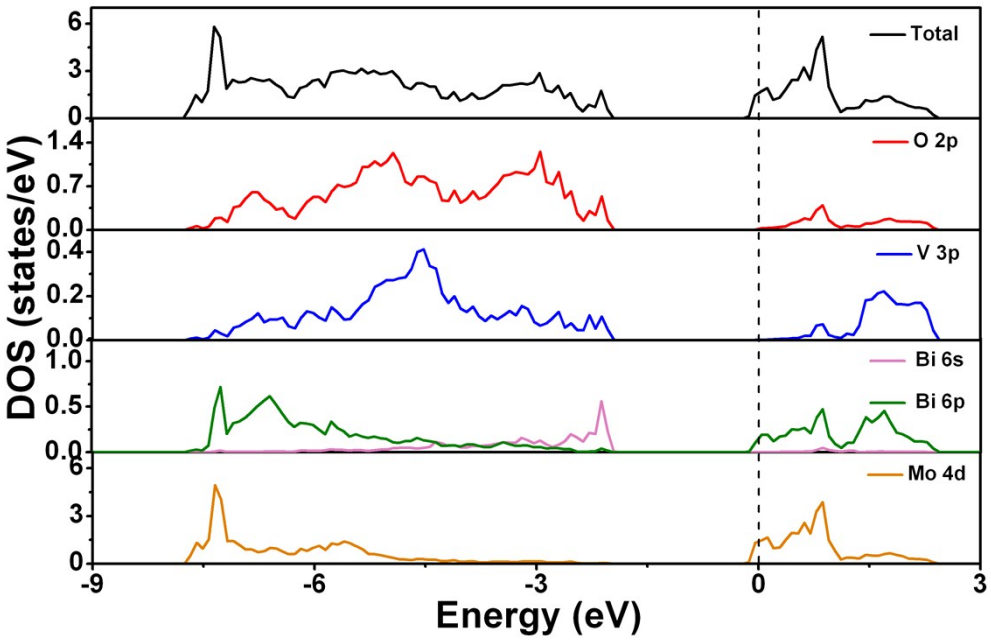


Fig. S6 Total DOS and the corresponding PDOSs of O2p, V3p, Bi 6s, Bi 6p, and Mo 4d states of Mo-BVO.

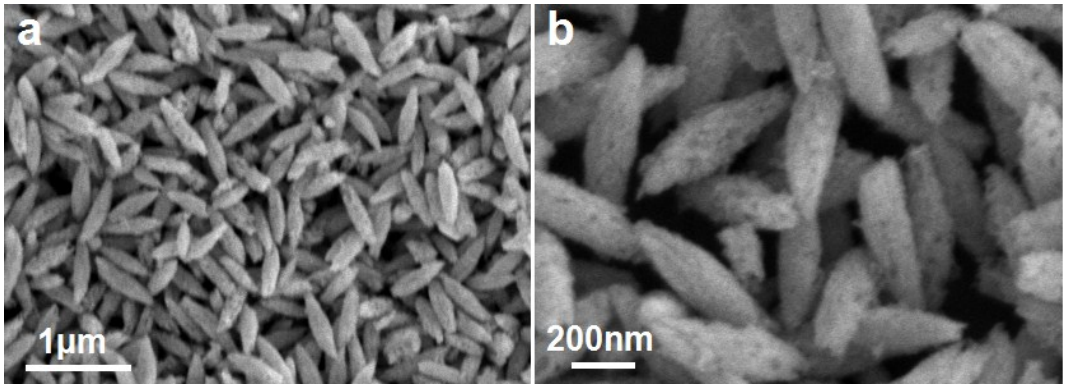


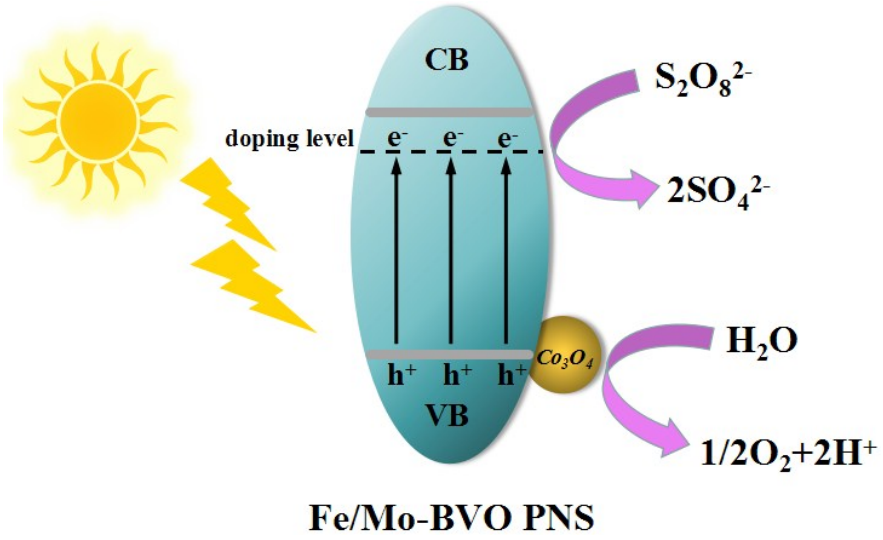
Fig. S7 SEM images of the as-prepared Fe/Mo-BVO PNSs after photocatalytic water oxidation test under visible-light irradiation.

Table S1 Relative VB and CB of all the photocatalysts calculated on the basis of Mott–Schottky plots

Photocatalysts	Band-gap (eV)	VB (V, *vs.* NHE)	CB (V, *vs.* NHE)
BVO	2.14	1.71	-0.43
Fe-BVO	1.93	1.63	-0.30
Mo-BVO	2.13	1.74	-0.39
Fe/Mo-BVO	1.87	1.73	-0.14

Table S2 A comparison study of the photocatalysts in this work and previous reported $BiVO_4$-based photocatalysts for water oxidation reaction.

Photocatalysts	Morphology	Light source	Wavelength	Sacrificial agents	O_2 evolution rate ($\mu mol\ g^{-1}\ h^{-1}$)	References
$Ca_{0.2}Bi_{0.8}V_{0.8}Mo_{0.2}O_4$	Not described	300 W Xe	>420 nm	$AgNO_3$	201.4	1
$BiVO_4$	Nanoparticle	300 W Xe	>420 nm	$FeCl_3$	108	2
$BiVO_4$	Rod-like nanostructure	300 W Xe	>300 nm	$AgNO_3$	82.8	3
Mo-$BiVO_4$	Nanoparticle	300 W Xe	≥420 nm	$AgNO_3$	500	4
Fe-$BiVO_4$	Nanoparticle	300 W Xe	≥420 nm	$AgNO_3$	<50	4
Y-$BiVO_4$	Rod-like microstructure	200-WHg-Xe	>300 nm	$AgNO_3$	285	5
BVO	Rugby-ball-like microstructure	300 W Xe	>420 nm	$NaOH/Na_2S_2O_8$	11	This work
Fe-BVO	Rugby-ball-like microstructure	300 W Xe	>420 nm	$NaOH/Na_2S_2O_8$	27	This work
Mo-BVO	Shuttle-like nanostructure	300 W Xe	>420 nm	$NaOH/Na_2S_2O_8$	125.1	This work
Fe/Mo-BVO	Shuttle-like nanostructure	300 W Xe	>420 nm	$NaOH/Na_2S_2O_8$	191.5	This work



Scheme S1 Schematic illustrating the mechanism of the as-prepared Fe/Mo-BVO PNS for water oxidation under visible-light irradiation.

References:

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