Supporting Information for

Bismuth Oxybromide Nanosheet as an Efficient Photocatalyst for Dye Degradation

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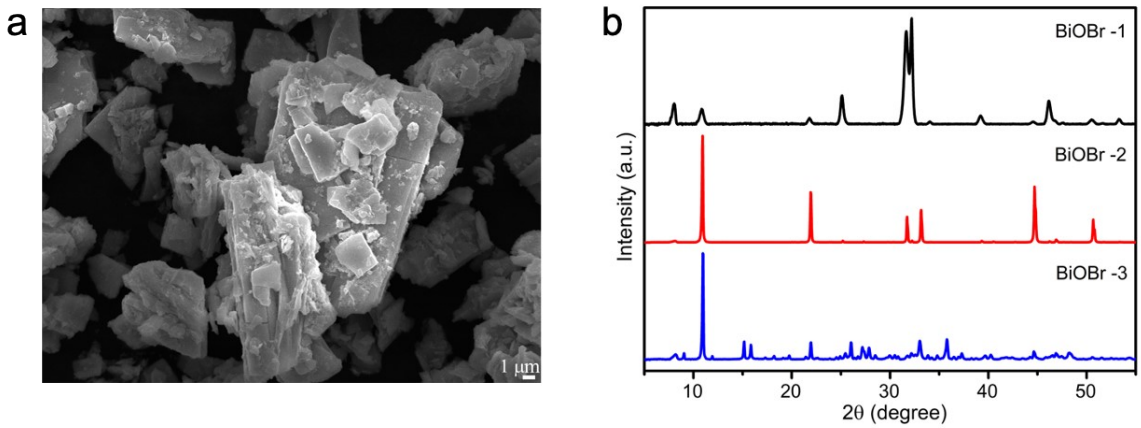

Figure S1. (a) SEM image of BiOBr-3. (b) Comparison of PXRD patterns of BiOBr.

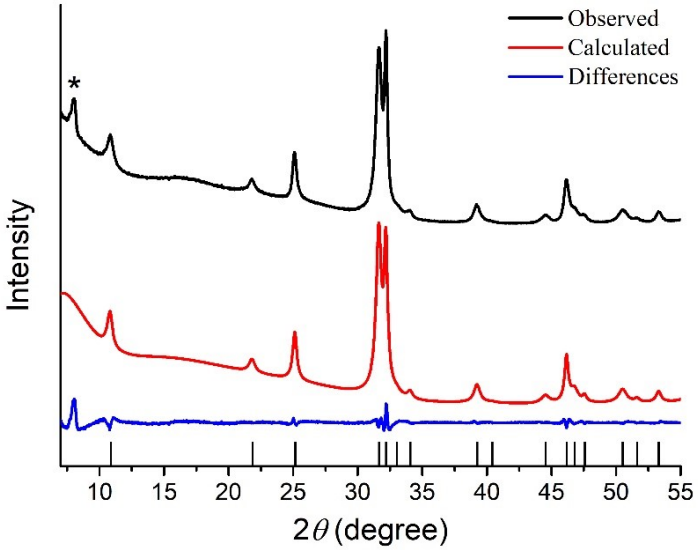

Figure S2. Pawley fitting against powder X-ray diffraction (λ = 1.5418Å) for BiOBr1. Red line: calculated; black line: observed; blue line: difference; black bars: Bragg conditions. Peaks marked with black stars in the observed pattern cannot be found in the simulated one. This peak should come from impurities during the synthesis.

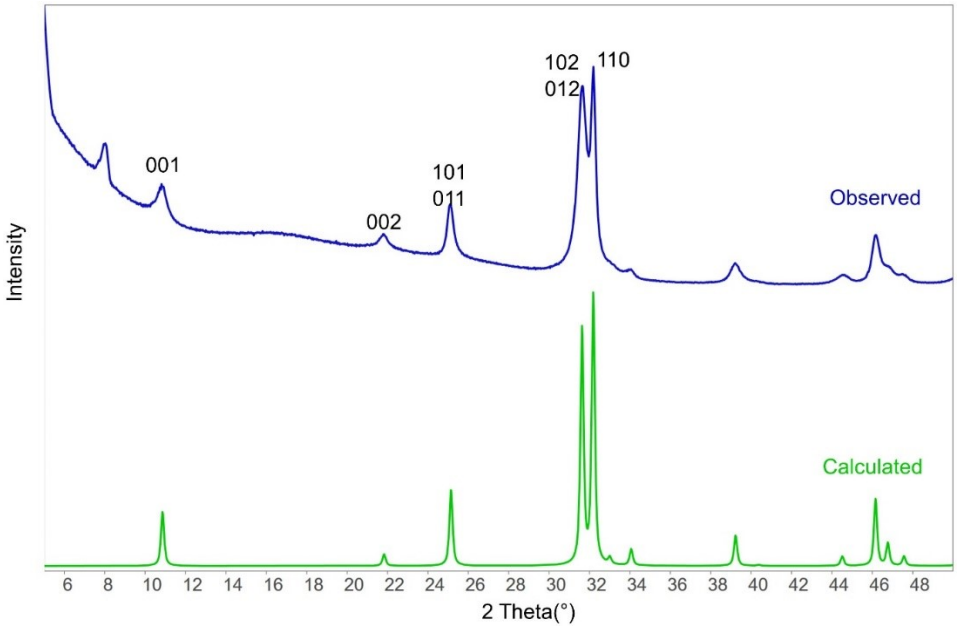

Figure S3. Simulated PXRD pattern (λ = 1.5418 Å) of BiOBr by using the structural model obtained from crystal structure solved by 3DED. It agrees well with the observed PXRD pattern.

Table S1. Single crystal data collection and crystallographic data for BiOBr (λ = 0.0251 Å).

Tilt range (°)	-53.0 to 61.3
Rotation angle (°)	114.3
Tilt rate (° s^{-1})	1.2
Exposure time per frame (s)	0.3
Total number of images	324
Data collection time (min)	1.6
Beam current (pA)	< 0.01

Table S2. Single crystal data collection and crystallographic data for BiOBr (λ = 0.0251 Å).

Chemical Formula	BiBrO
Formula weight	304.88
Crystal system	Tetragonal
Space Group	$P4/nmm$
a (Å)	4.1750(8)
b (Å)	4.1750(8)
c (Å)	8.5700(17)
α (°)	90

β (°)	90
γ (°)	90
Volume	149.38(6)
Z	2
Wavelength (Å)	0.0251
Temperature (K)	293(2)
Completeness (%)	74.0
No. of reflections (all unique)	88
No. of reflections (Fo>4σ(Fo))	530
Refined parameters	6
R_{int}	0.2836
R_1 (Fo>2σ(Fo))	0.2571
R_1 (all reflections)	0.2635
GOF	3.458

Table S3. Crystallographic details of Pawley fitting of BiOBr.

Crystal system	Tetragonal
Space group	$P4/nmm$
a (Å)	3.9280(3)
b (Å)	3.9280(3)
c (Å)	8.128(1)
α (°)	90.0
β (°)	90.0
γ (°)	90.0
Volume (Å^3)	125.4(0)
wavelength (Å)	1.5406
R_p (%)	3.1
Rw_p (%)	4.4
R_{exp} (%)	1.2
GOF	3.6

References

(1) Cichocka, M. O.; Ångström, J.; Wang, B.; Zou, X.; Smeets, S. High-Throughput Continuous Rotation Electron Diffraction Data Acquisition via Software Automation. *J Appl Cryst* **2018**, *51* (6), 1652–1661. https://doi.org/10.1107/S1600576718015145.
(2) Kabsch, W. XDS. *Acta Cryst D* **2010**, *66* (2), 125–132. https://doi.org/10.1107/S0907444909047337.