

Electronic Supplementary Information (ESI)

First-Principles Studies on Facet-Dependent Photocatalytic Properties of Bismuth Oxyhalides (BiOXs)

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Table S1. Bi-O/Bi-X Bonds Lengths for Different BiOX Structures (in Å).

Terminations	BiOF	BiOCl	BiOBr	BiOI
Bulk	2.298/3.498	2.333/3.945	2.343/4.127	2.362/4.303
{001}-1X	Surface	2.300/3.423	2.334/3.957	2.347/4.130
	Central	2.298/3.498	2.333/3.950	2.344/4.133
{001}-2X	Surface	2.340/3.191	2.345/3.890	2.344/4.137
	Central	2.291/3.490	2.333/3.948	2.344/4.113
{001}-BiO	Surface	2.327/3.605	2.355/3.849	2.311/4.093
	Central	2.291/3.490	2.333/3.949	2.345/4.113
{110}-O	Surface	2.204/3.588	2.185/3.849	2.157/4.096
	Central	2.291/3.490	2.333/3.948	2.344/4.113
{110}-BiX	Surface	2.253/3.588	2.276/3.719	2.290/3.826
	Central	2.291/3.490	2.333/3.948	2.344/4.113
{010}	Surface	2.282/3.468	2.296/3.847	2.294/3.889
	Central	2.301/3.586	2.319/3.945	2.339/4.109