

Electronic supplementary information

**Oxyhalides: Prospecting Ore for Optical Functional Materials
with Large Laser Damage Thresholds**

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Figure S1 Density of states (DOS) and the specific orbitals in the energy range near the band gaps for Sr_4OCl_6 (a), Ba_4OCl_6 (b), Ba_2OBr_2 (c), BiOCl (d), $\text{Bi}_3\text{O}_4\text{Br}$ (e), $\text{Bi}_4\text{O}_5\text{Br}_2$ (f), $\text{Bi}_5\text{O}_7\text{Br}$ (g), $\text{Bi}_7\text{O}_5\text{F}_{11}$ (h) and $\text{Bi}_{24}\text{O}_{31}\text{Cl}_{10}$ (i).





