Supporting Information

"XA_6" Octahedra Influencing the Arrangement of Anionic Groups and Optical Properties in Inverse-Perovskite $[B_6O_{10}]XA_3$ (X=Cl, Br; A=alkali metal)

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Electronic Supplementary Information:

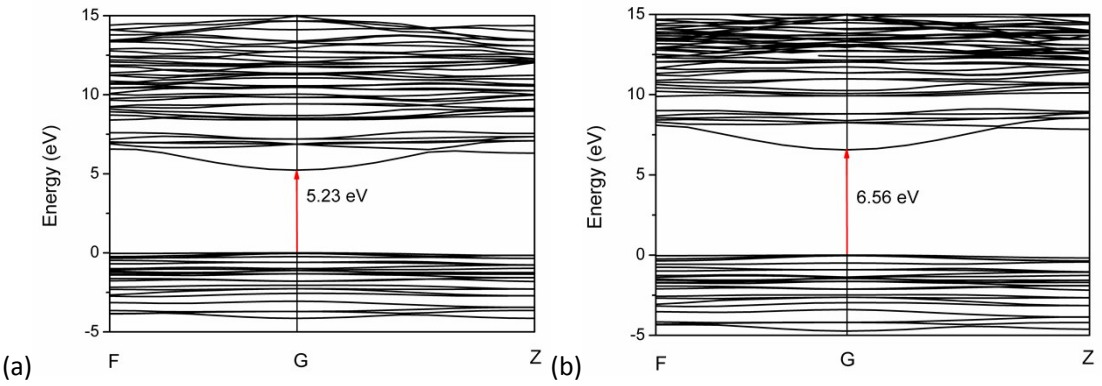

Figure S1. The band structures of α-RBOC calculated by GGA+PBE (a) and HSE06 (b).

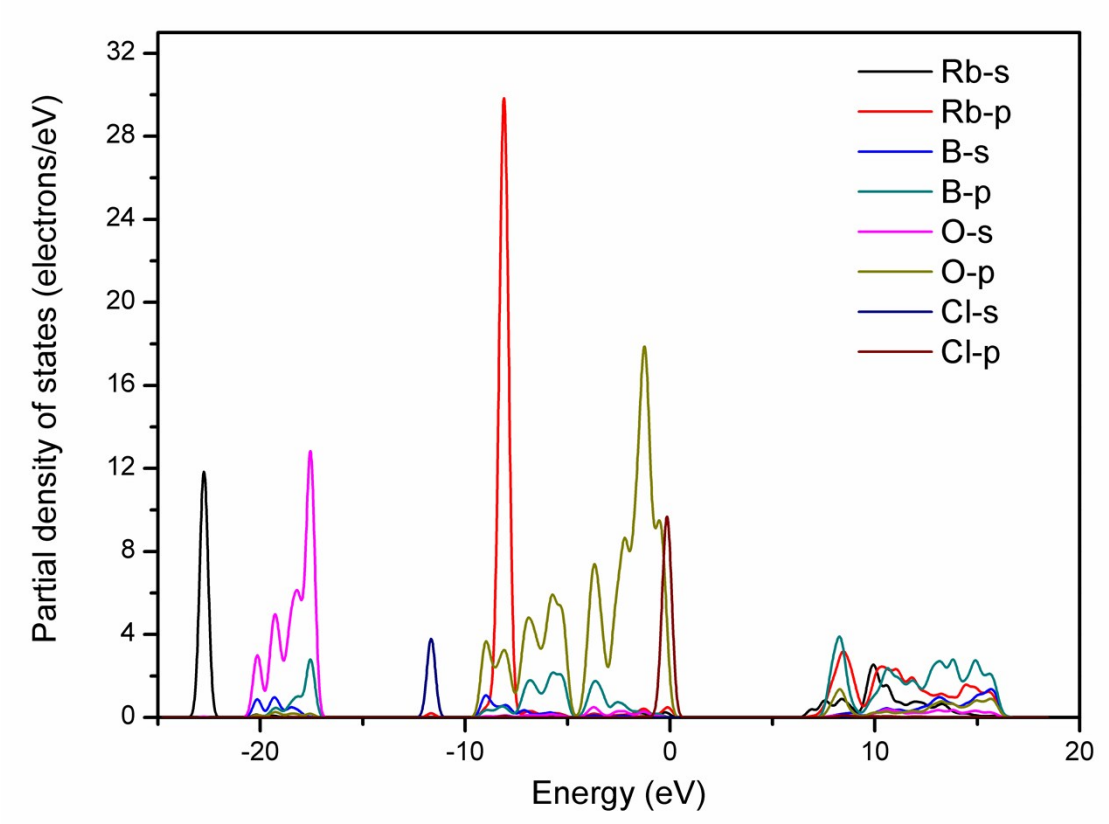

Figure S2. The partial density of states (PDOS) of α-RBOC.

Table S1. The lattice constants of α-RBOC

Compound	α-RBOC
Space group	R3m
Crystal system	Trigonal
a = b (Å)	10.271
c (Å)	9.221
α=β(°)	90
γ (°)	120
Volume (Å3)	842.494

Table S2. Independent elastic constants C_{ij}, bulk, shear, Young's moduli (B, G and E all in GPa), Poisson's ratio *v* and the ratio B/G of α-RBOC.

Crystal	C_{11}	C_{33}	C_{44}	C_{12}	C_{13}	C_{14}	C_{15}	B	G	E	*v*	B/G
α-RBOC	130.6	62.5	40.9	36.4	45.2	45.1	0	57.1	36.1	x=y=93.0 Z=38.0	xy=yx=0.085 xz=yz=0.661 zx=zy=0.270	1.59