Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Theoretical and experimental investigations of BiOCl for electrochemical adsorption of cesium ions

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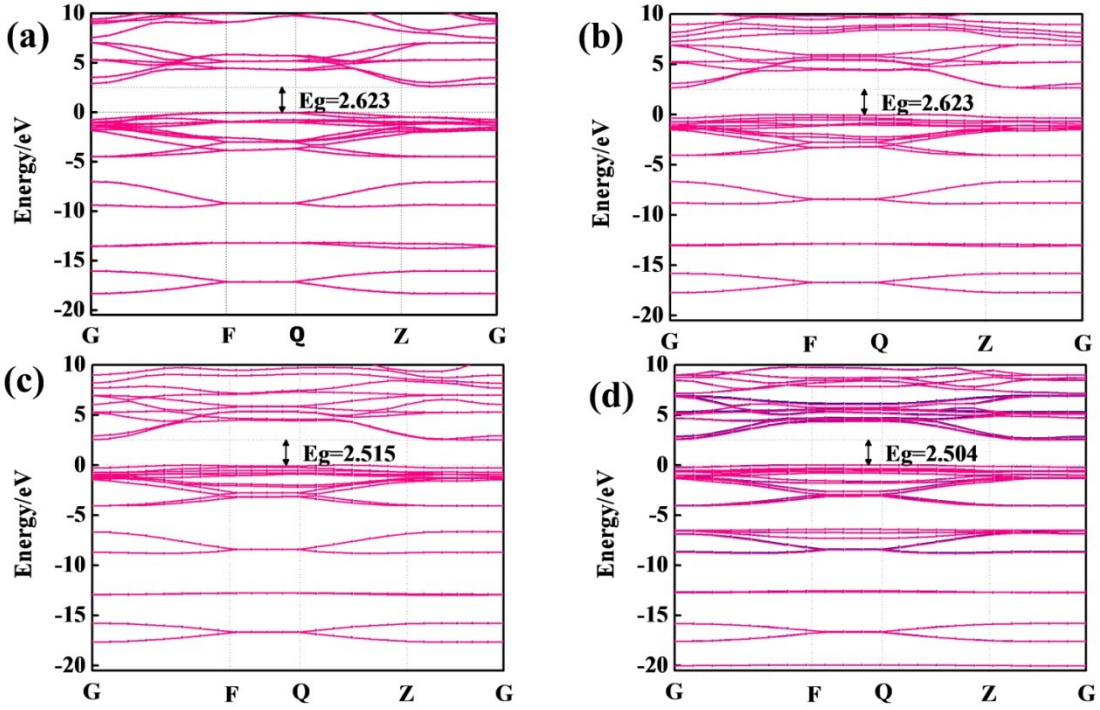

Fig. S1 The band structures of (a) BiOCl, (b) Li-BiOCl, (c) Na-BiOCl and (d) Cs-BiOCl crystals.

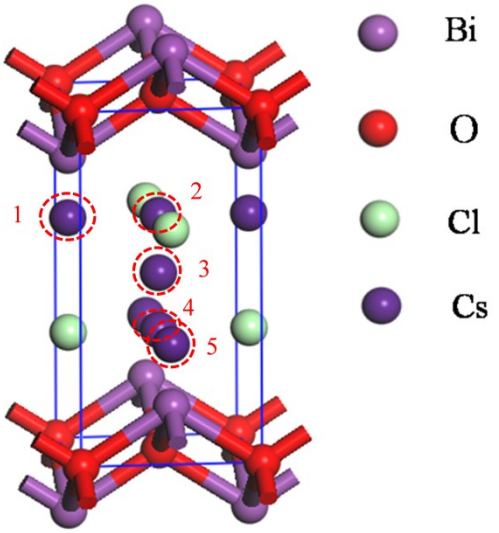

Fig. S2 The five initial adsorption sites in BiOCl crystal.

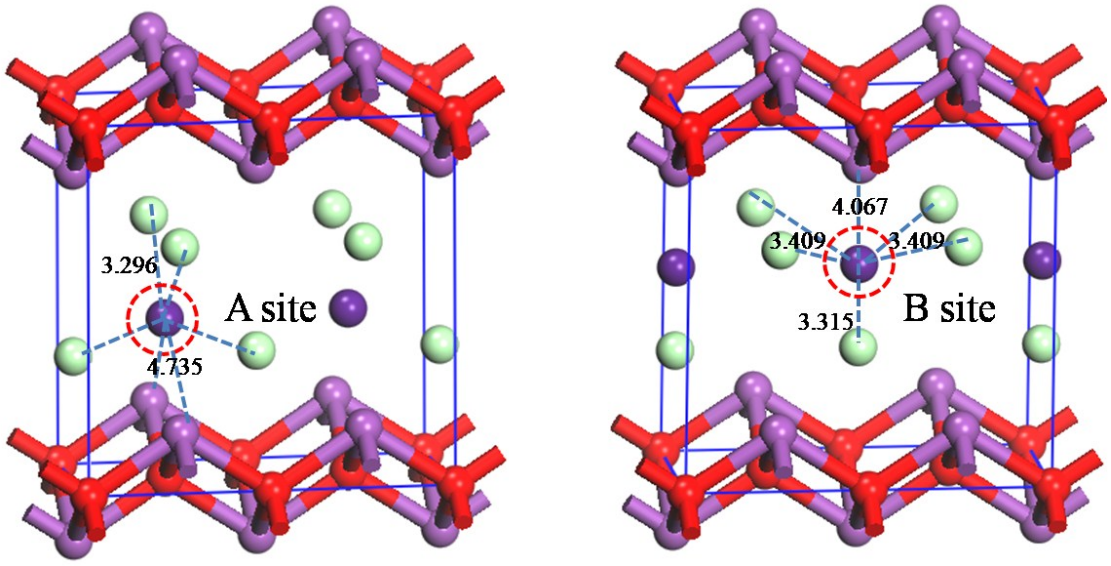

Fig. S3 The optimized structures and distance (Å) of Cs (A)-BiOCl (left) and Cs (B)-BiOCl (right).

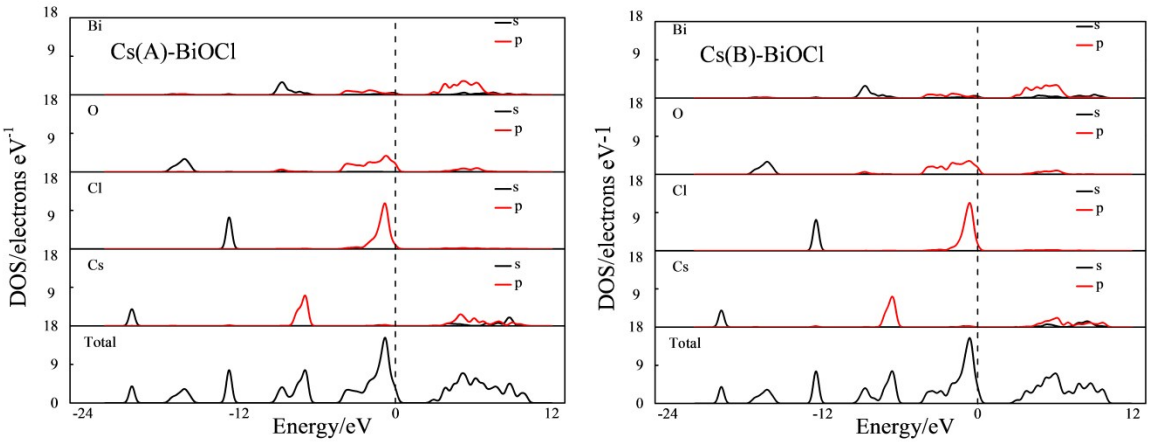

Fig. S4 DOS and PDOS of Cs (A)-BiOCl (left) and Cs (B)-BiOCl (right). The dashed lines indicate Fermi level.

Table S1 Binding energy (eV) of three ions at the five initial adsorption sites in BiOCl crystal.

Initial adsorption sites	Binding energy		
	Li (eV)	Na (eV)	Cs (eV)
1	-0.67641	-0.2039	-1.95338
2	-1.12582	-0.36591	-1.89892
3	-1.12307	-0.36622	-1.89447
4	-1.12583	-0.36574	-1.89695
5	-0.67562	-0.20306	-1.95234

Table S2 The calculated atomic Mulliken charge population for BiOCl and Cs-BiOCl.

Species	Mulliken charge population (e)			
	Bi	Cl	O	Cs
BiOCl	1.42	-0.52	-0.9	-
Cs-BiOCl	1.14	-0.655	-0.87	0.72

Table S3 Magnetic momentum (Unit: μB) of pure BiOCl, Li-BiOCl, Na-BiOCl, and Cs-BiOCl.

Species	Magnetic momentum (μB)			
	Bi	Cl	O	Li, Na or Cs
BiOCl	0	0	0	-
Li-BiOCl	0	0	0	0
Na-BiOCl	0	0	0	0
Cs-BiOCl	-0.2	0	0	-0.02