## **Supporting Information**

## Theoretical calculation assisted materials screening of BiOX (X =

## F, Cl, Br, I) for electrochemical absorption of cesium ions

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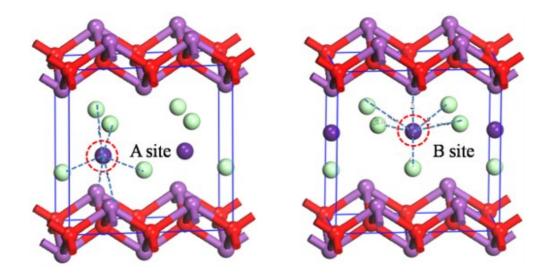


Fig. S1 The difference of A site and B site in BiOX crystal.

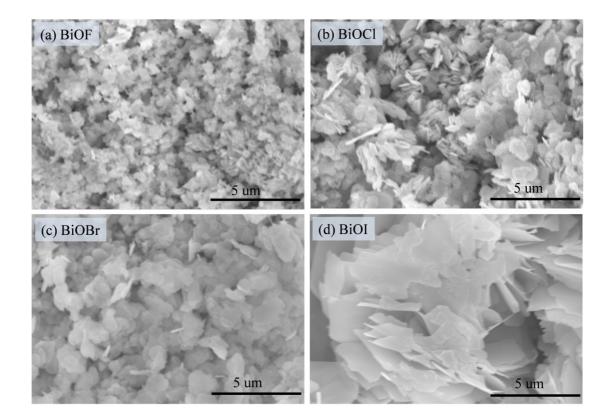


Fig. S2 The SEM images of (a) BiOF, (b) BiOCl, (c) BiOBr, and (d) BiOI.

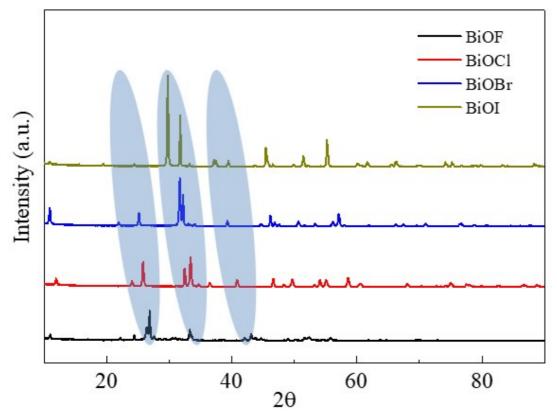
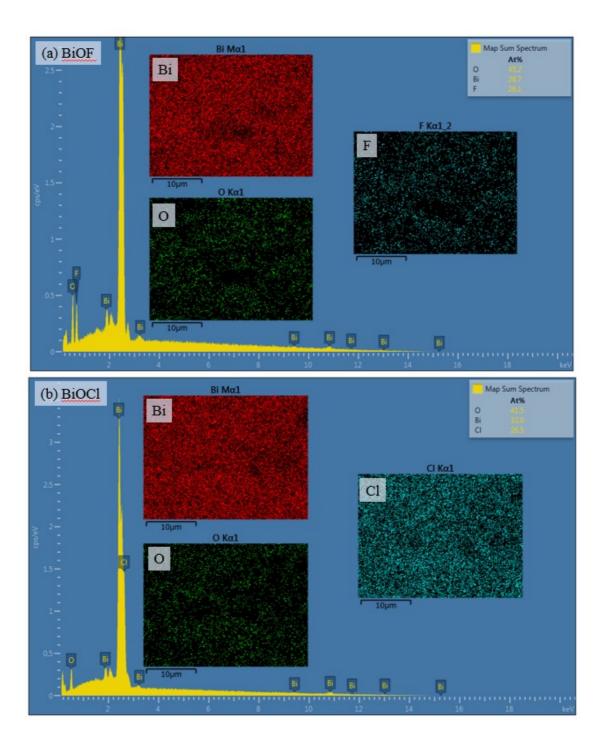


Fig. S3 The XRD patterns of BiOF, BiOCl, BiOBr, and BiOI.



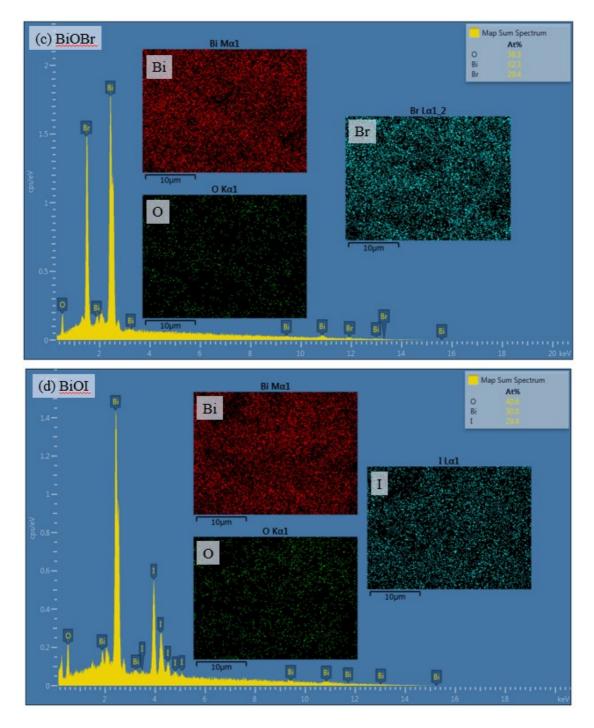


Fig. S4 The EDS results of (a) BiOF, (b) BiOCl, (c) BiOBr, and (d) BiOI.