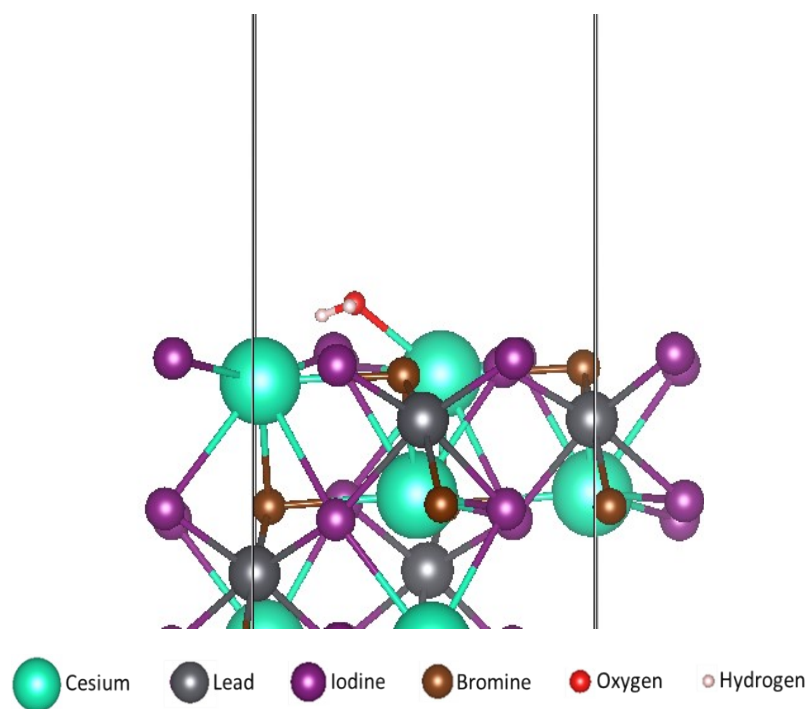


Fig. S1 Time evolution of the O-H distance of water molecule on (001) CsPbI₂Br/H₂O interface.

(a)



(b)

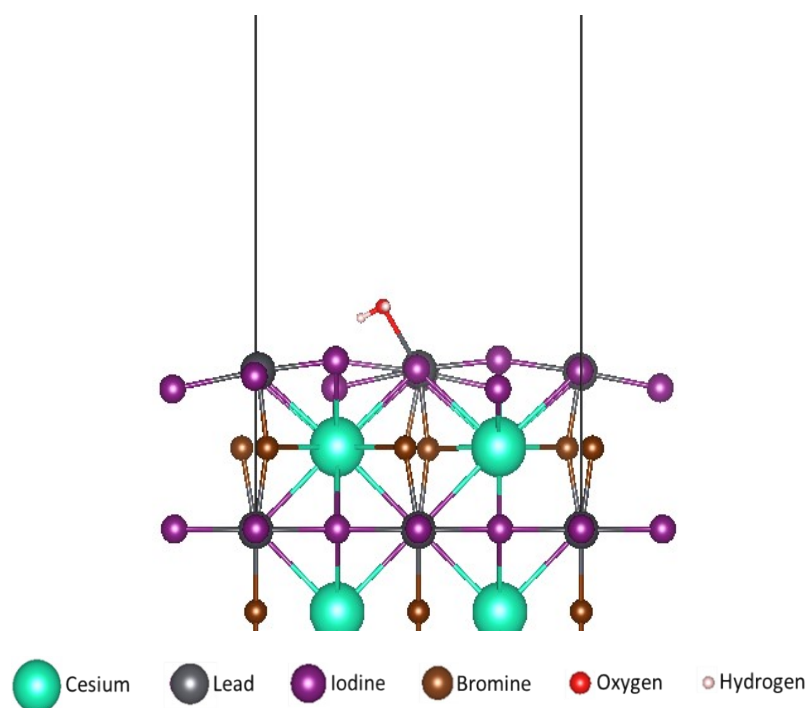
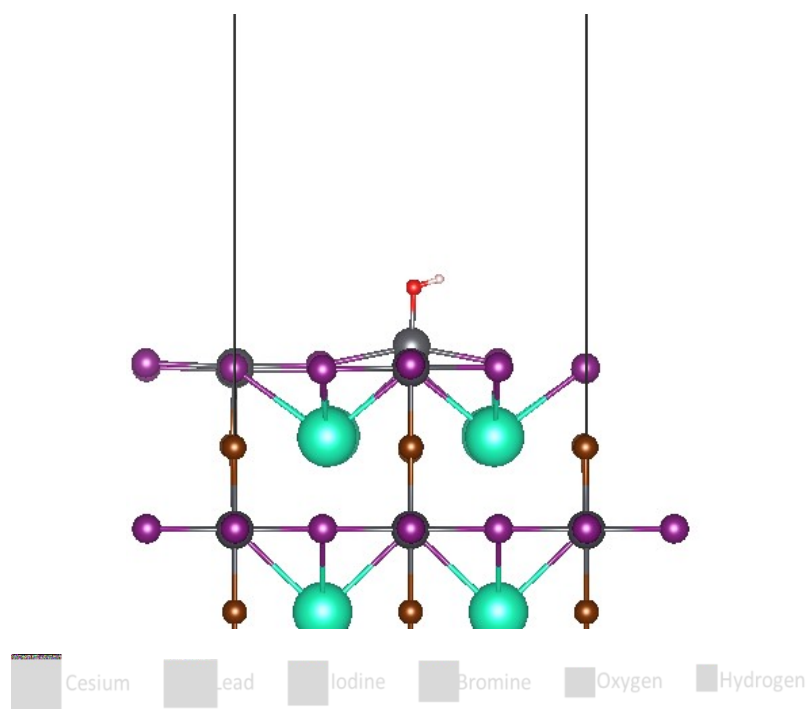


Fig S2: Water adsorption on the (a) (111) and (b) 001 surface of CsPbI₂Br

(a)



(b)

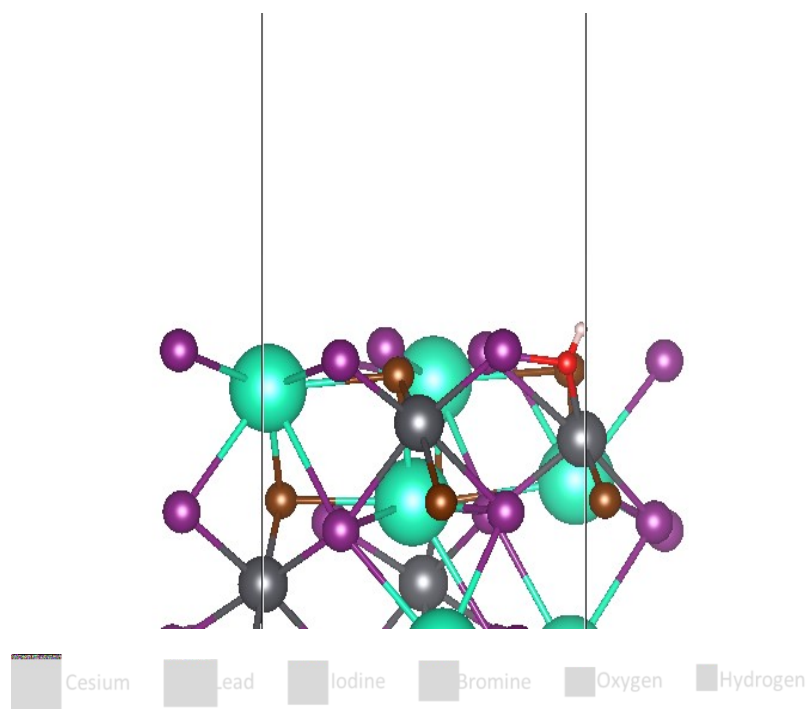
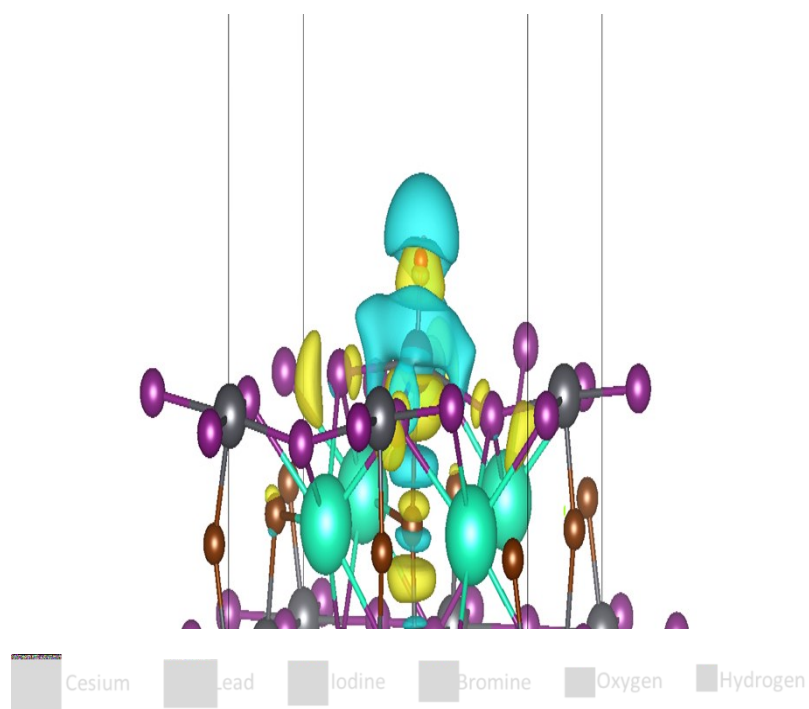


Fig S3 OH⁻ adsorbed on the (a) (001) surface of CsPbI₂Br and (b) (111) surface of CsPbI₂Br

(a)



(b)

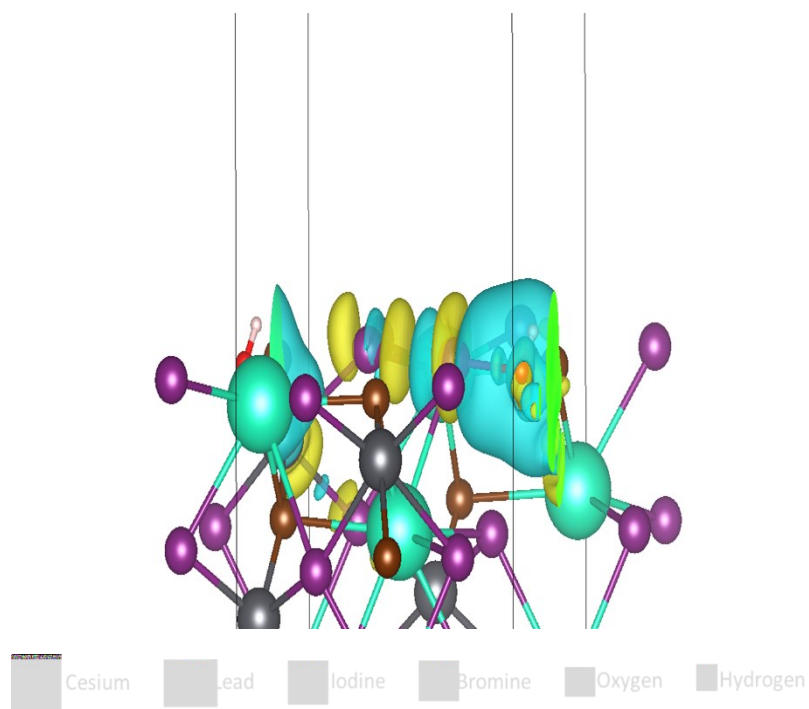


Fig S4 Charge density difference (CDD) plots of OH⁻ on (a) (001) plane of CsPbI₂Br and (b) (111) plane of CsPbI₂Br