Supporting Information：

Thickness-induced band-gap engineering in lead-free double perovskite $Cs_2AgBiBr_6$ for highly efficient photocatalysis

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Figure S1

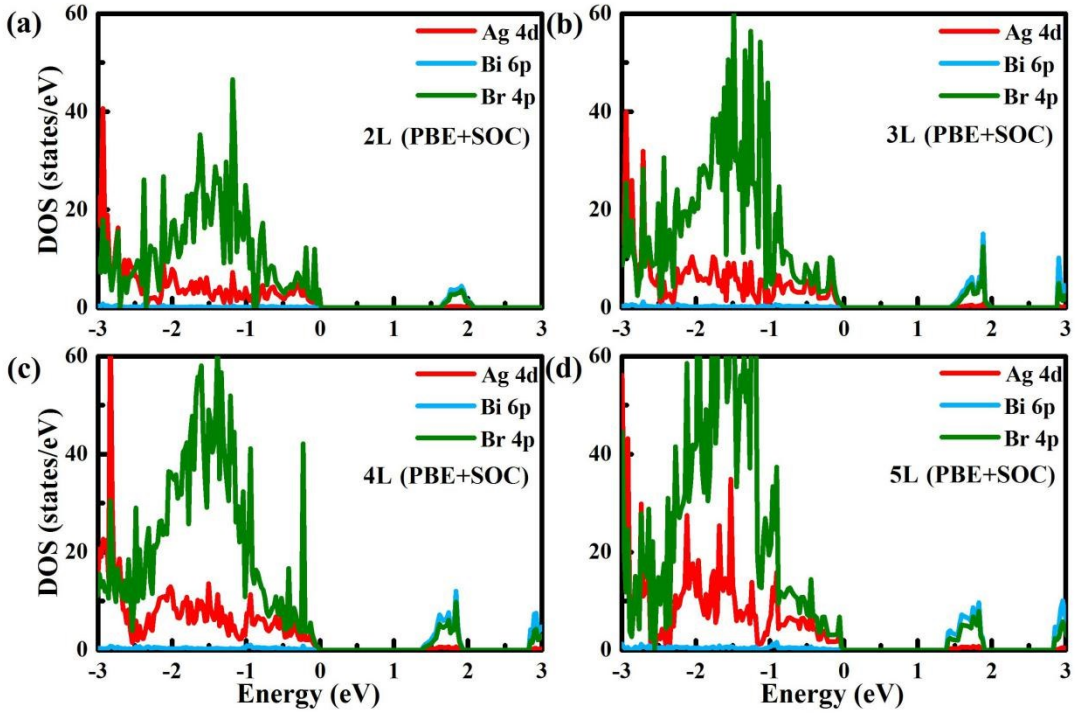

Fig. S1 Calculated projected density of states (PDOS) of $Cs_2AgBiBr_6$ with PBE+SOC functional for (a) two-layer, (b) three-layer, (c) four-layer and (d) five-layer configurations. The Fermi level is set at 0 eV.

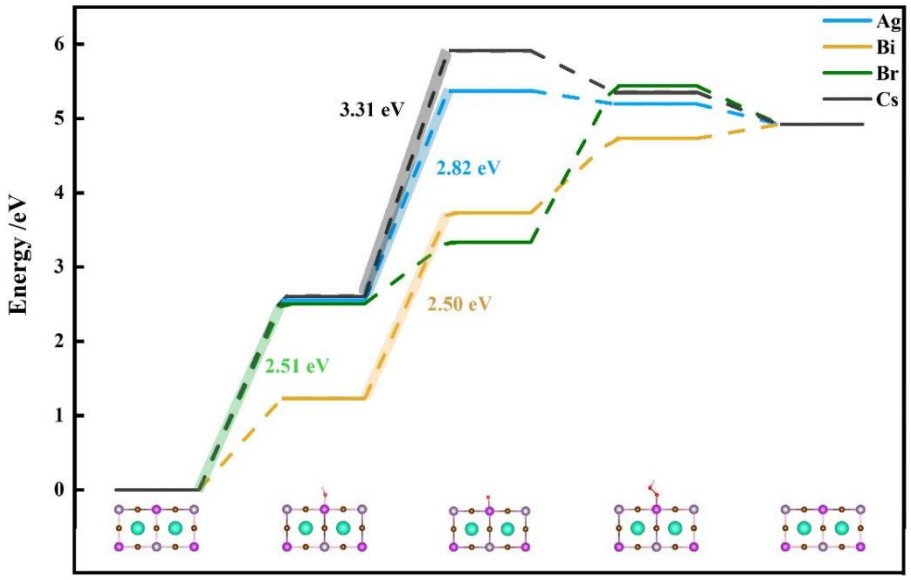

Figure S2 Free energy diagram at 0 V for OER of the different sites of single-layer $Cs_2AgBiBr_6$.The highlights indicate the rate-determining step with the values of the limiting energy barrier labelled.

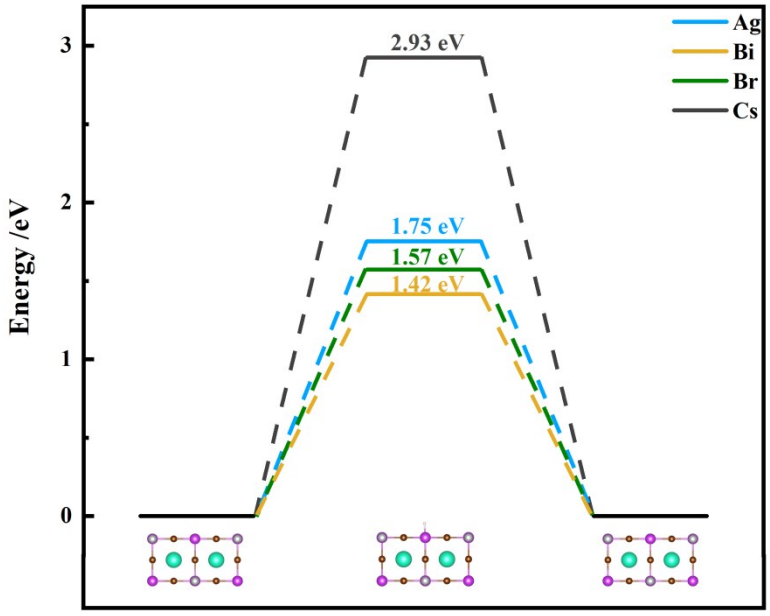

Figure S3 Free energy diagram at 0 V for HER of the different sites of single-layer $Cs_2AgBiBr_6$.

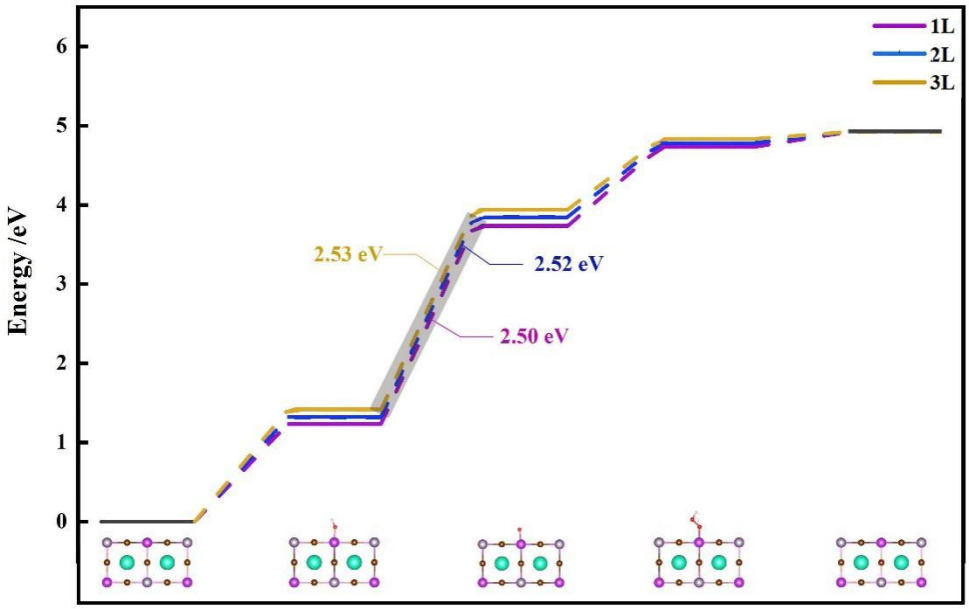

Figure S4 Free energy diagram at 0 V for OER of the different layers of $Cs_2AgBiBr_6$.The highlights indicate the rate-determining step with the values of the limiting energy barrier labelled.

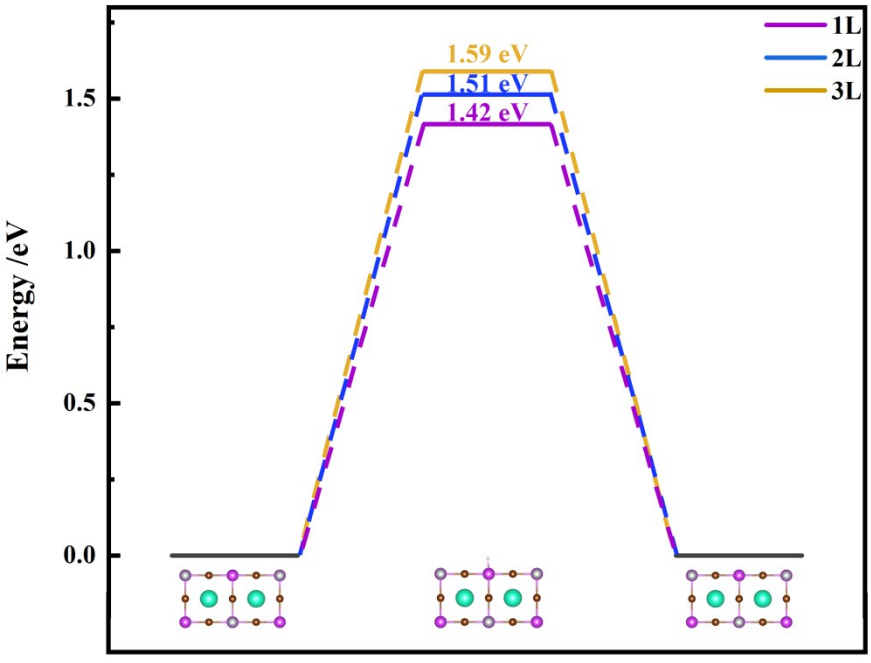

Figure S5 Free energy diagram at 0 V for HER of the different layers of $Cs_2AgBiBr_6$.

Table S1

Table S1 Calculated band gaps (eV) of the halide double perovskite $Cs_2AgBiBr_6$ with different thicknesses by PBE, PBE+SOC and HSE+SOC functional.

Layer	PBE	PBE+SOC	HSE+SOC
1L	2.02	1.53	2.39
2L	1.82	1.53	2.36
3L	1.56	1.31	2.11
4L	1.48	1.28	2.09
5L	1.44	1.22	2.04