Supplementary Material

# Adhesion, stability, structural and electronic properties of perovskite/$BaWO_4$ heterostructures: First-principles and experimental characterizations

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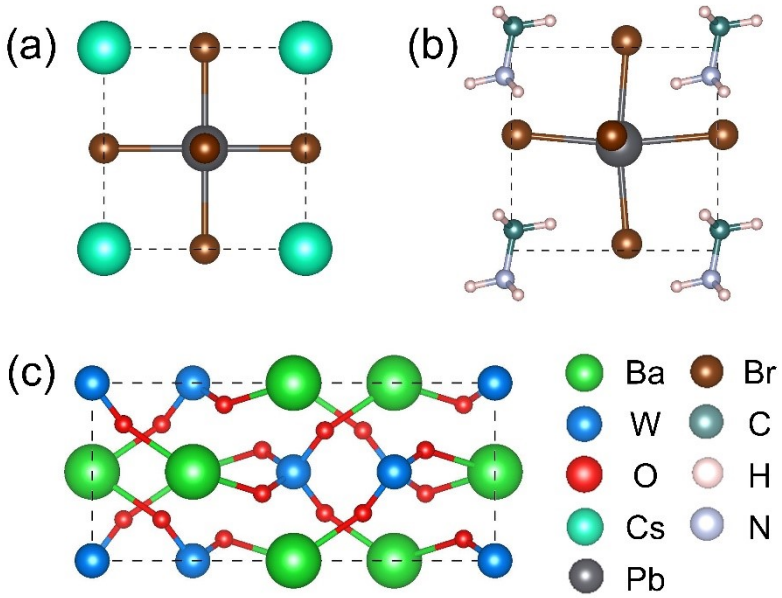
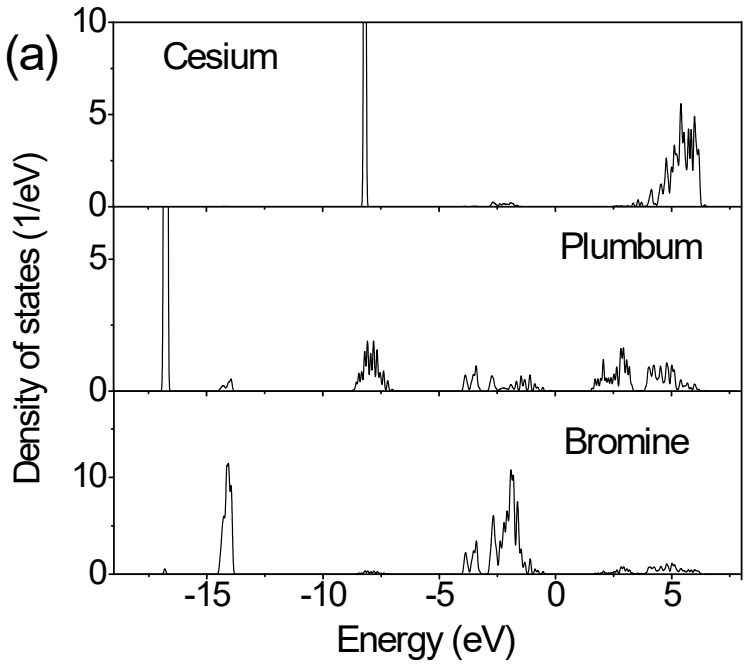
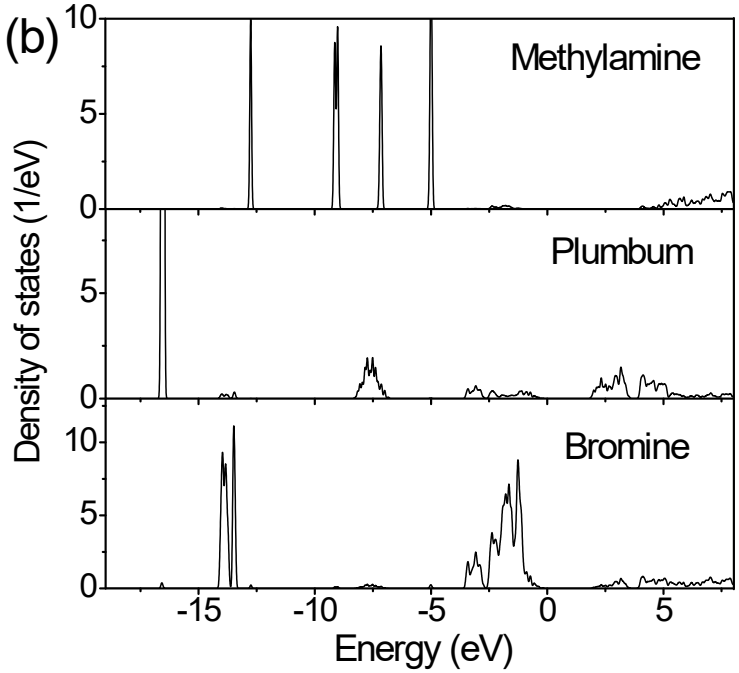


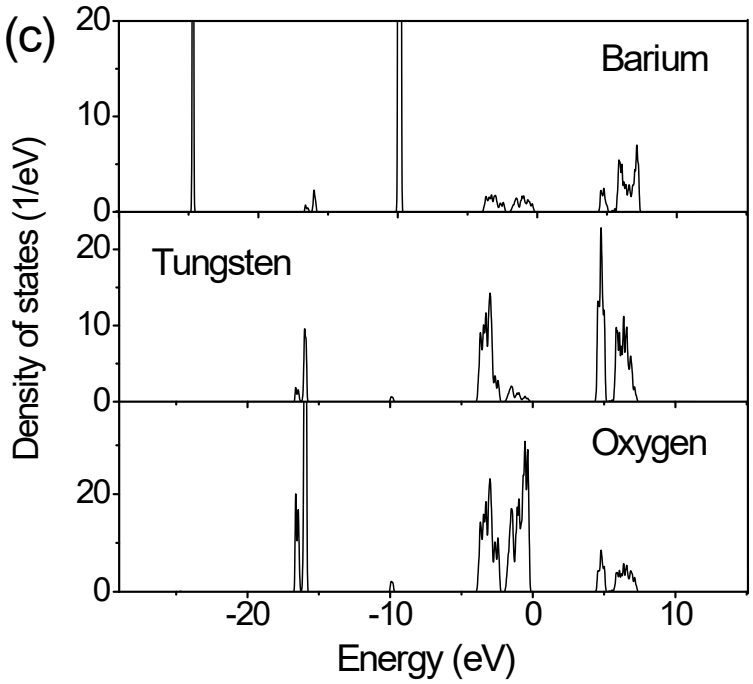

**Figure S1** Crystal structures of (a) cubic $CsPbBr_3$, (b) monoclinic $MAPbBr_3$, and (c) tetragonal $BaWO_4$.


(a)
Cesium
Plumbum
Bromine
Density of states (1/eV)
Energy (eV)
10
5
0
5
0
10
0
-15
-10
-5
0
5

1


(b)
Methylamine
Plumbum
Bromine
Density of states (1/eV)
Energy (eV)
10
5
0
5
0
10
5
0
-15
-10
-5
0
5

2

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2 **Figure S2** DOS of (a) cubic $CsPbBr_3$, (b) monoclinic $MAPbBr_3$, and (c) tetragonal

3 $BaWO_4$ in bulk phase.

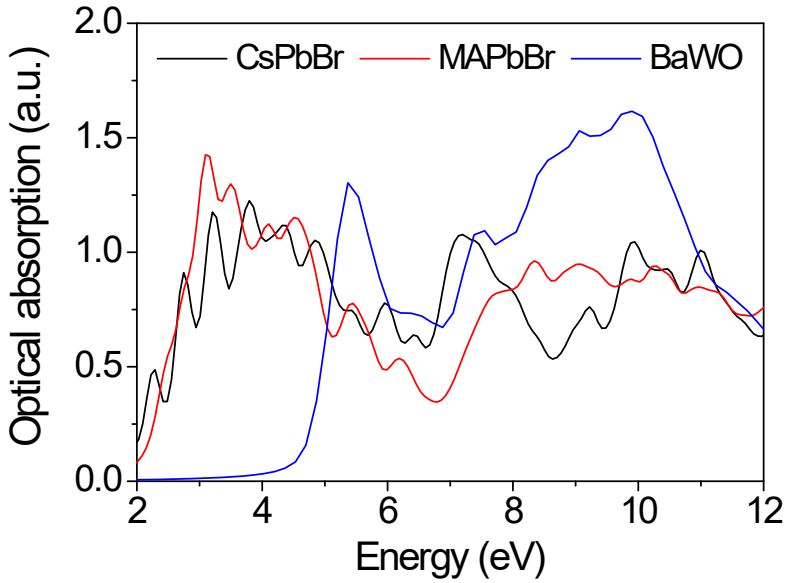


**Figure S3** Absorption coefficients of cubic $CsPbBr_3$, monoclinic $MAPbBr_3$, and tetragonal $BaWO_4$ in bulk phase.

**Table S1** Calculated lattice parameters (Å) of cubic $CsPbBr_3$, monoclinic $MAPbBr_3$, and tetragonal $BaWO_4$.

| | *a* | *b* | *c* |
|---|---|---|---|
| $CsPbBr_3$ | 6.00 | 6.00 | 6.00 |
| $MAPbBr_3$ | 6.04 | 6.06 | 6.13 |
| $BaWO_4$ | 5.71 | 5.71 | 12.94 |

**Table S2** Lattice parameters (Å) and mean absolute strain (%) of $CsPbBr_3/BaWO_4$ and $MAPbBr_3/BaWO_4$ models.

| | $CsPbBr_3/BaWO_4$ | $MAPbBr_3/BaWO_4$ |
|---|---|---|
| lattice parameter *a* | 5.85 | 5.88 |
| lattice parameter *b* | 12.45 | 12.59 |
| Mean absolute strain | 2.08 | 1.89 |