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


# Supporting Information

# Electronic Structure of $CsPbBr_{3-x}Cl_x$ Perovskites: Synthesis, Experimental Characterization, and DFT Simulations

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Table S 1: The photoluminescence color coordinates in CIE 1931 color space before and after 60 s exposure to severe UV light.

| Sample No. | Segregation | CIE (x; y) | |
|---|---|---|---|
| | | 0.05 s | 60 s |
| 1 | no | 0.101; 0.799 | 0.101; 0.799 |
| 2 | yes | 0.034; 0.651 | 0.054; 0.708 |
| 3 | yes | 0.069; 0.250 | 0.068; 0.682 |
| 4 | yes | 0.129; 0,069 | 0,082; 0,506 |
| 5 | yes | 0.151; 0.026 | 0.083; 0.708 |
| 6 | no | 0.171; 0.005 | 0.171; 0.005 |

Table S 2: The example of relative atomic coordinates in the unit cell depicted in Fig. S4 used in ab-initio calculations of $CsPbBr_{3-x}Cl_x$ perovskites.

| | x (Å) | y (Å) | z (Å) |
|---|---|---|---|
| Cs | 4.913120749 | 0.163683846 | 0.008249258 |
| Cs | 0.808635503 | 3.842198963 | 0.013122274 |
| Pb | 0.140292860 | -0.089041763 | 2.925429046 |
| Pb | 4.263047731 | 4.013372255 | 2.921214821 |
| Br | 0.009171368 | -0.919140542 | 0.008759922 |
| Br | 4.172242932 | 4.879404747 | 0.010271223 |
| Br | 2.640089438 | 1.515107050 | 2.338832585 |
| Br | 6.764593007 | 2.426344372 | 2.343228667 |
| Br | 1.755855871 | 5.616882652 | 3.496413927 |
| Br | 5.864141171 | 6.497840794 | 3.542465185 |
| Cs | 3.582925978 | -0.314134036 | 5.825674006 |
| Cs | -0.509218555 | 4.220891544 | 5.829913789 |
| Pb | 0.141159585 | -0.086300863 | 8.729075689 |
| Pb | 4.264024166 | 4.015965462 | 8.735347170 |
| Br | 0.261523527 | 0.762267465 | 5.826896738 |
| Br | 4.367730147 | 3.146574698 | 5.828186009 |
| Br | 2.639193072 | 1.519979087 | 9.318884985 |
| Br | 6.767370263 | 2.431166478 | 9.311993969 |
| Br | 1.759430092 | 5.622618828 | 8.155753468 |
| Br | 5.863954059 | 6.501733752 | 8.113296746 |

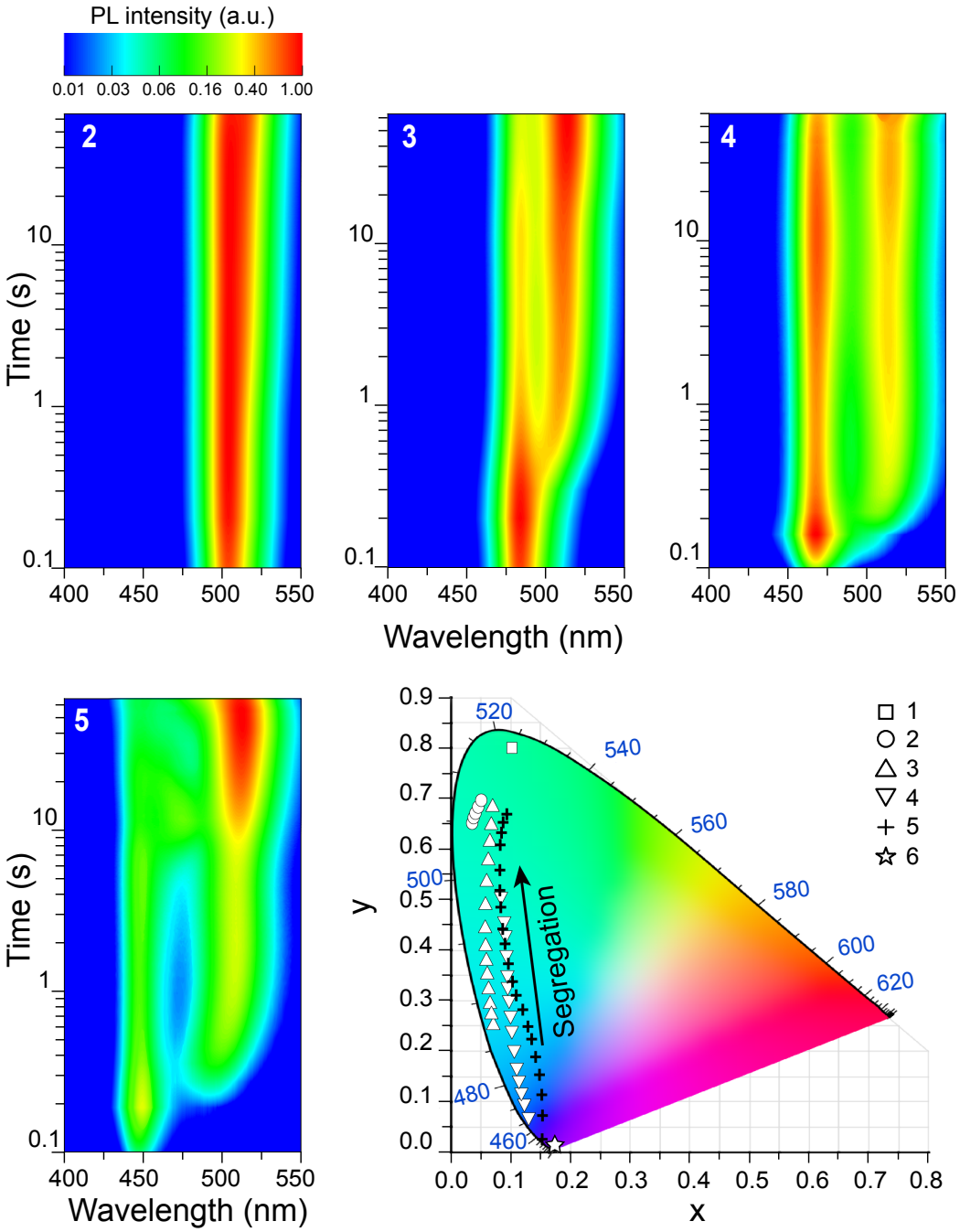


Figure S 1: PL dynamics caused by light-induced halide ion segregation in mixed-halide perovskite thin films and its representation in CIE 1931 color space.

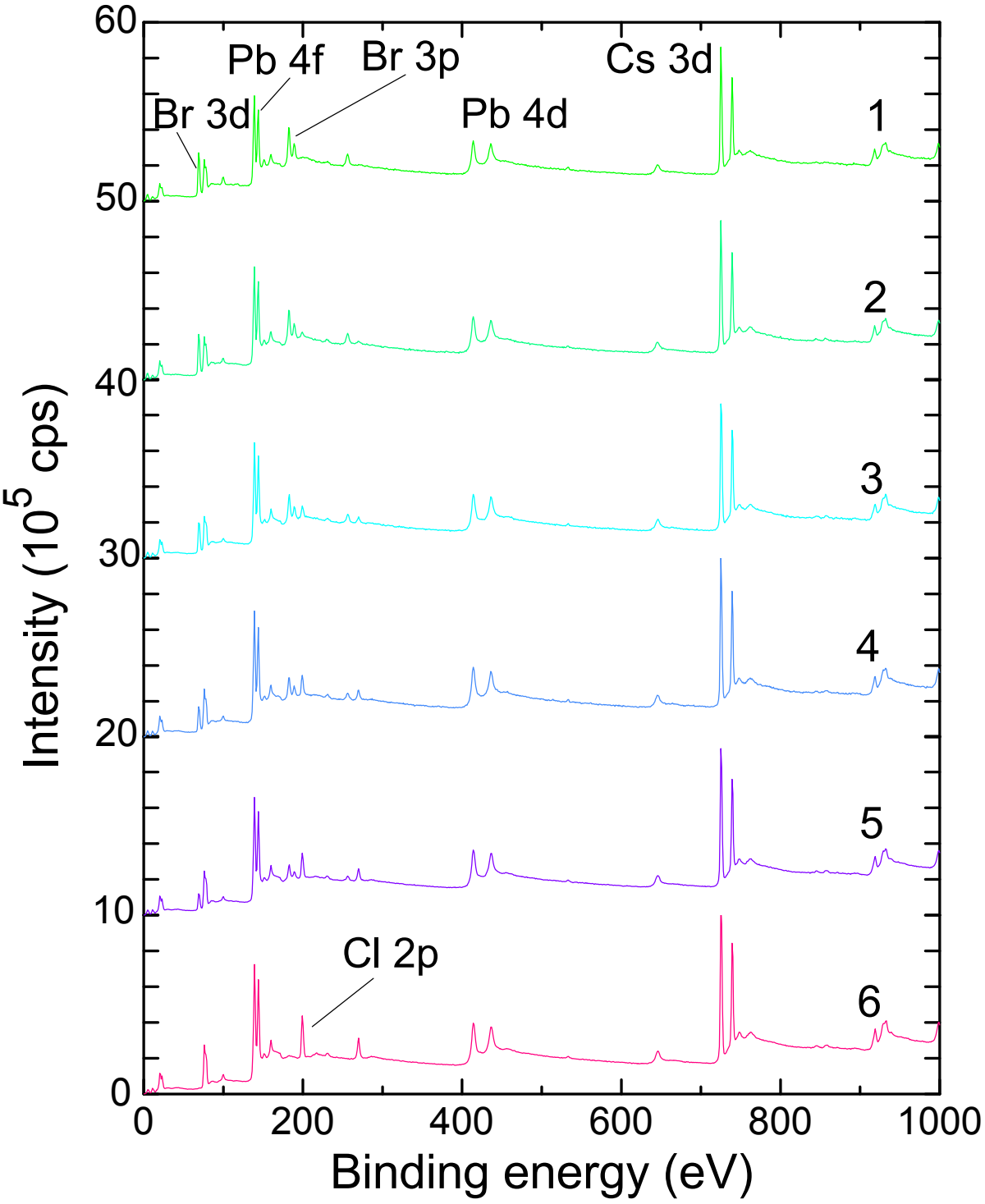


Figure S 2: Survey scan XPS spectra for **1-6**

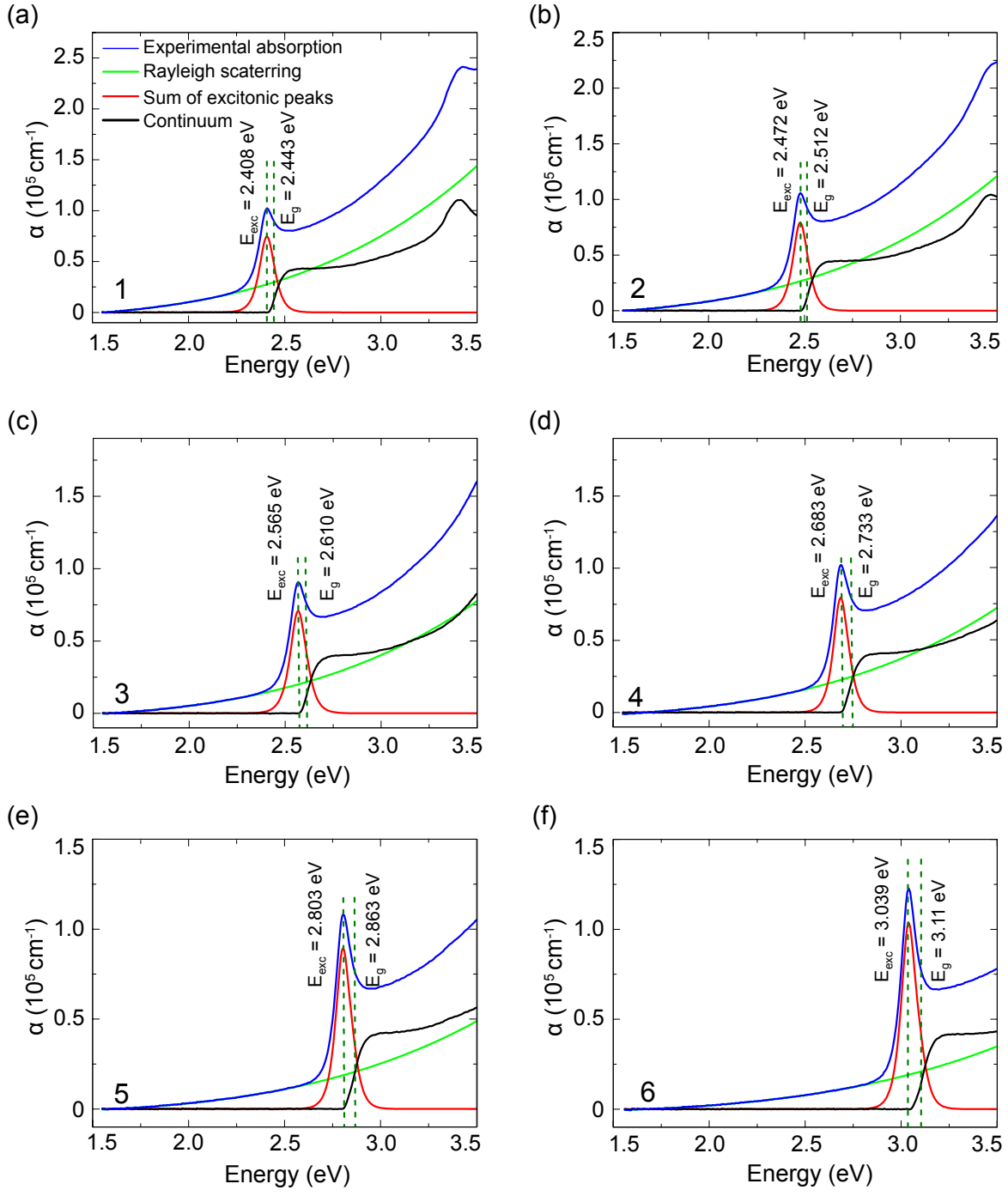


Figure S 3: Spectral deconvolution of the experimental extinction of **1**-**6**. Continuum stands for band-to-band electronic absorption.

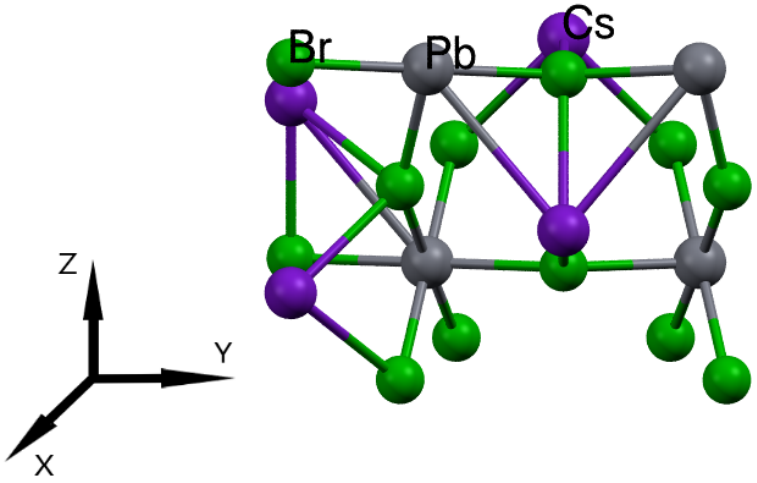


Figure S 4: The example of the orthorombic unit cell (Pnma) used in the ab-initio calculations. The atomic coordinates are presented in the Table S2

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