Is Cs$_2$TiBr$_6$ a promising Pb-free perovskite for solar energy applications?

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SUPPLEMENTARY INFORMATION

Figure S1. XRD spectra of Cs$_2$TiBr$_6$ powder without thermal treatment before and directly after removal of the protective Kapton film. The dashed lines denote the peak position of the lower lattice constant Cs$_2$TiBr$_6$ phase. The relative humidity RH is around 45-50 % during the measurement.
Figure S2. Pawley profile fitting of the XRD pattern of Cs$_2$TiBr$_6$ powder annealed at 100°C for 30 min. Goodness of fit, $R_p$ and $R_w$ values of 0.99, 9.54 and 12.91 are extracted from the Pawley fitting, respectively. The resulting refined unit cell parameter is $a = 10.6907\pm0.0005$ Å.

Figure S3. Tauc plots for Cs$_2$TiBr$_6$ considering indirect and direct bandgaps. The data are acquired using diffuse reflectance measurements on Cs$_2$TiBr$_6$ powder.
**Figure S4.** a) Absorption spectra obtained from successive diffuse reflectance measurements on Cs₂TiBr₆ powder. Each measurement takes about 5 min. b) Tauc plots considering indirect and direct bandgaps on the 3rd measurement in a) (orange).

**Figure S5.** PL spectrum of Silicon substrate using an excitation wavelength of 442 nm.
Figure S6. Evolution of the Cs₂TiBr₆ PL spectra between the first (directly after exposure to ambient atmosphere) and after and the second (after ~3 min) measurement.

Figure S7. Imaginary part of the dielectric function $\varepsilon_2$ around the fundamental band edge obtained from DFT calculations.
Figure S8. Evolution of Cs$_2$TiBr$_6$ XRD spectra over time in ambient atmosphere with a relative humidity RH around 45-50%.