

Is Cs_2TiBr_6 a promising Pb-free perovskite for solar energy applications?

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SUPPLEMENTARY INFORMATION

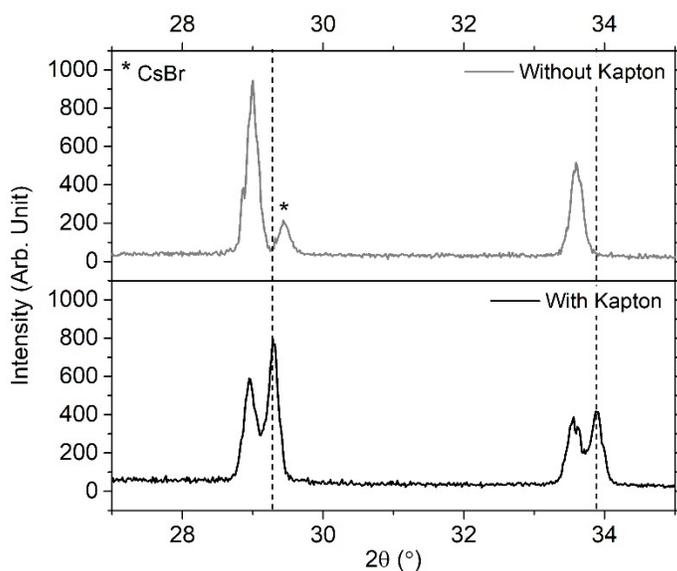


Figure S1. XRD spectra of Cs_2TiBr_6 powder without thermal treatment before and directly after removal of the protective Kapton film. The dashed lines denote the peak position of the lower lattice constant Cs_2TiBr_6 phase. The relative humidity RH is around 45-50 % during the measurement.

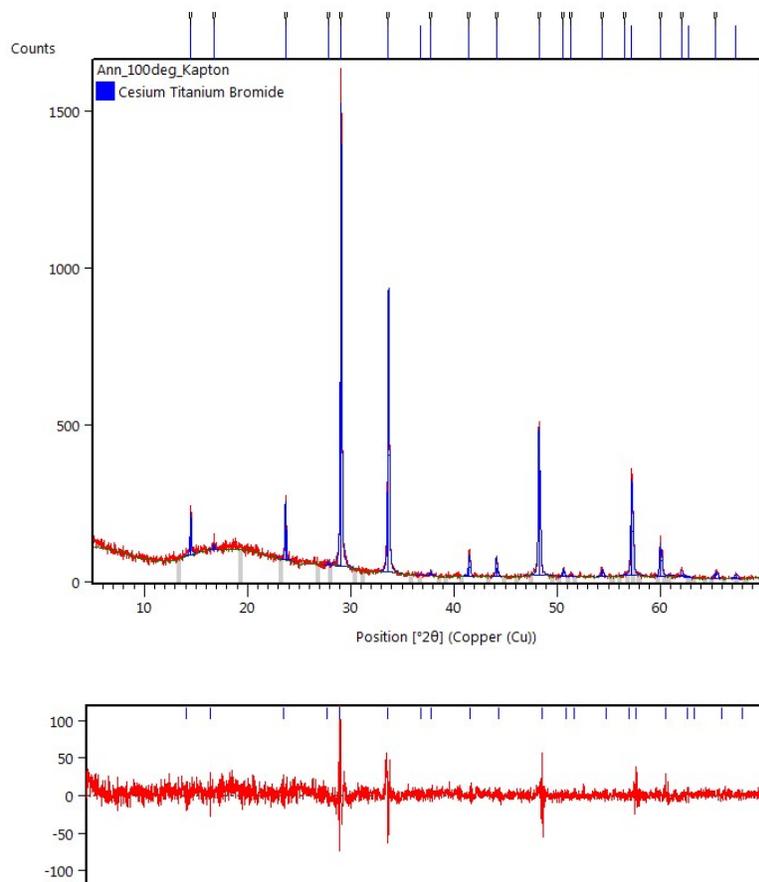


Figure S2. Pawley profile fitting of the XRD pattern of Cs_2TiBr_6 powder annealed at 100°C for 30 min. Goodness of fit, R_p and R_w values of 0.99, 9.54 and 12.91 are extracted from the Pawley fitting, respectively. The resulting refined unit cell parameter is $a = 10.6907 \pm 0.0005 \text{ \AA}$.

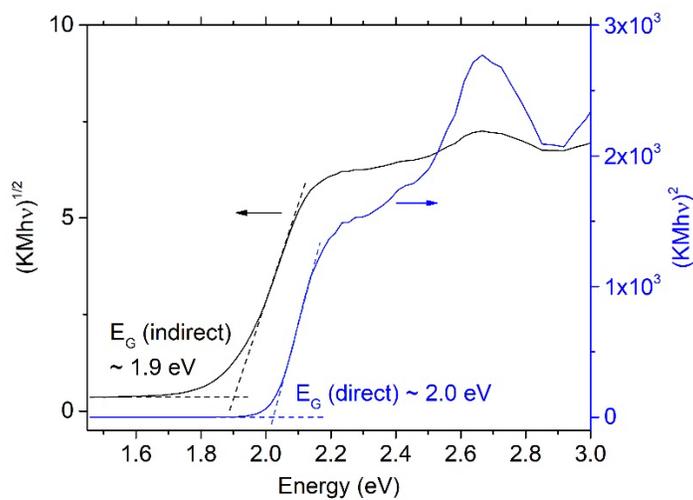


Figure S3. Tauc plots for Cs_2TiBr_6 considering indirect and direct bandgaps. The data are acquired using diffuse reflectance measurements on Cs_2TiBr_6 powder.

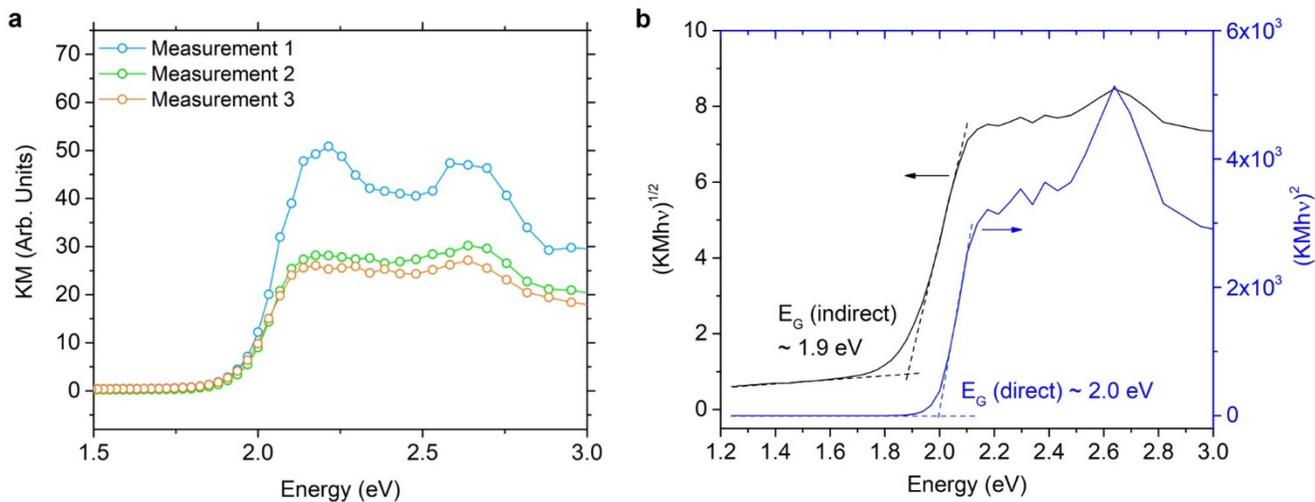


Figure S4. a) Absorption spectra obtained from successive diffuse reflectance measurements on Cs₂TiBr₆ powder. Each measurement takes about 5 min. b) Tauc plots considering indirect and direct bandgaps on the 3rd measurement in a) (orange).

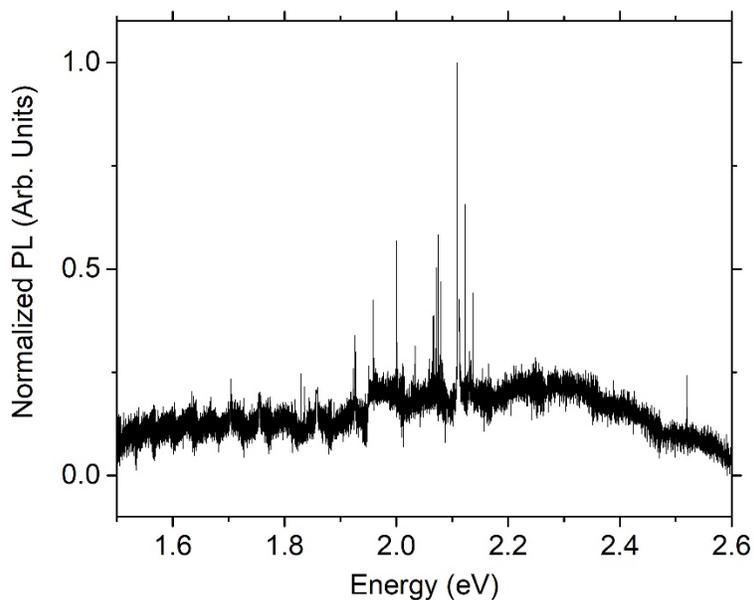


Figure S5. PL spectrum of Silicon substrate using an excitation wavelength of 442 nm.

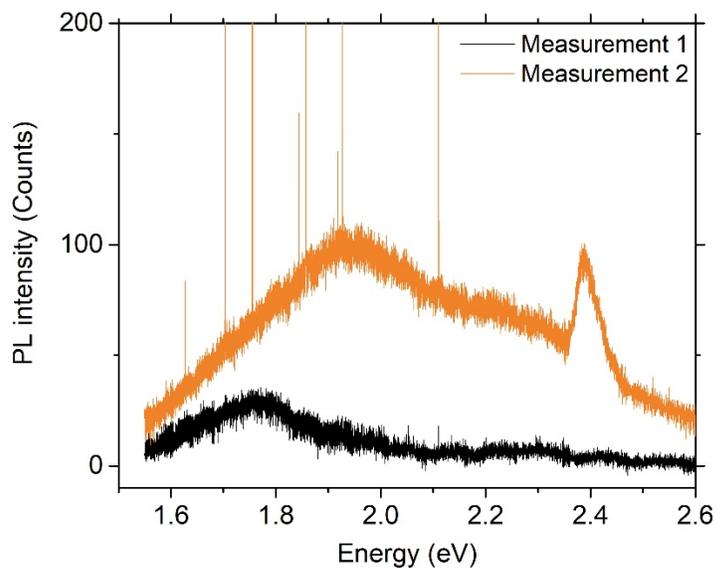


Figure S6. Evolution of the Cs_2TiBr_6 PL spectra between the first (directly after exposure to ambient atmosphere) and after the second (after ~ 3 min) measurement.

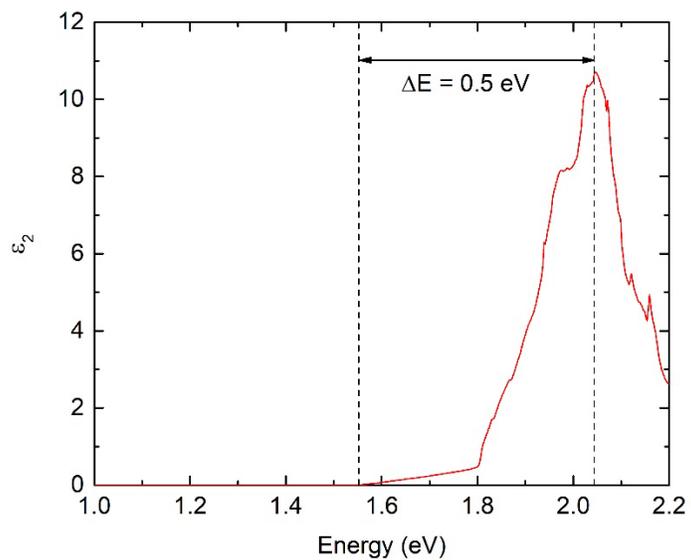


Figure S7. Imaginary part of the dielectric function ϵ_2 around the fundamental band edge obtained from DFT calculations.

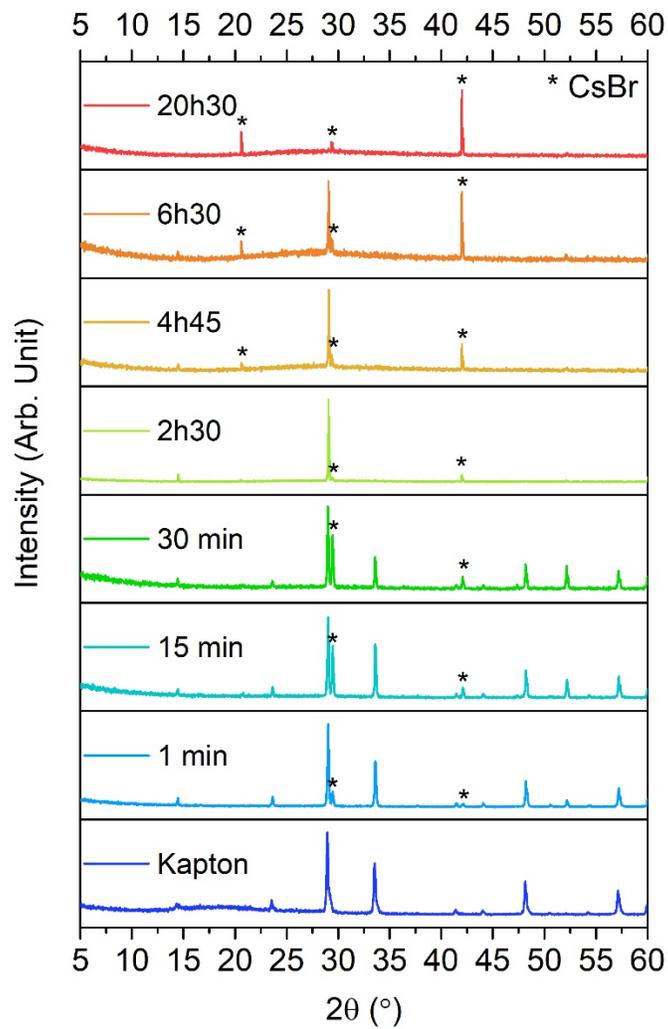


Figure S8. Evolution of Cs_2TiBr_6 XRD spectra over time in ambient atmosphere with a relative humidity RH around 45-50%.