Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.
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Stability investigation of the titanium-based eco-friendly perovskite-like antifluorite Cs_2TiBr_6

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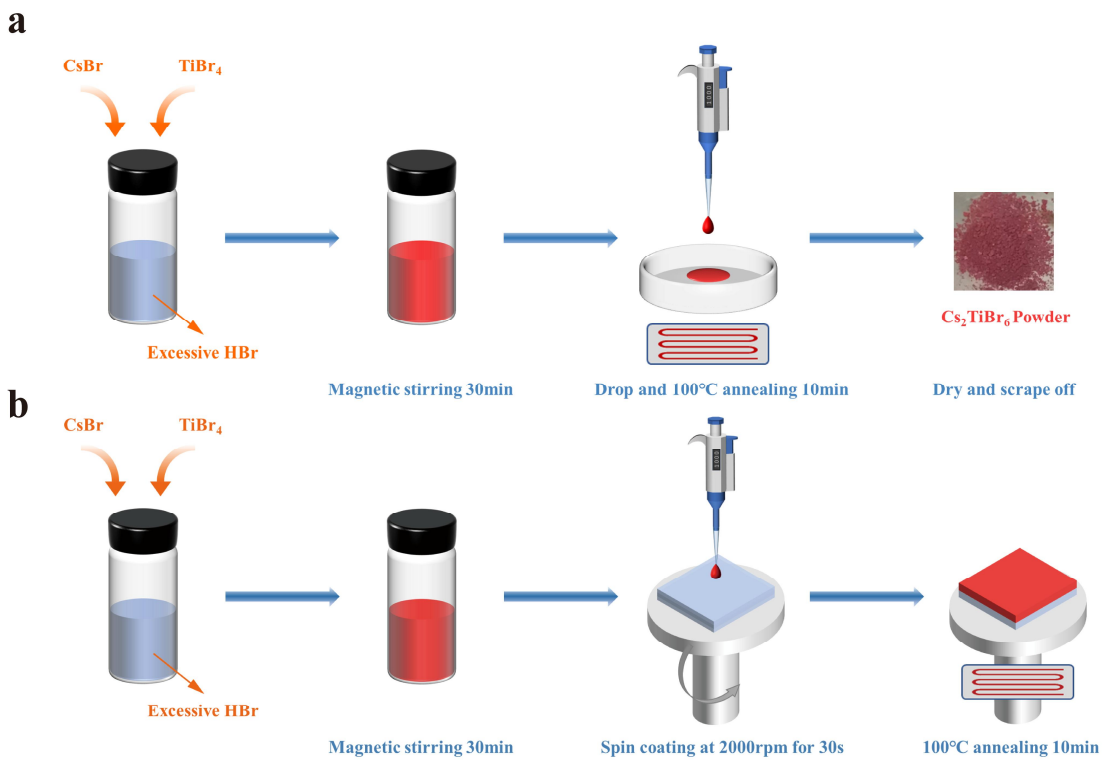

Figure S1 Schematic of the preparation for the Cs_2TiBr_6 (a) powder and (b) film.

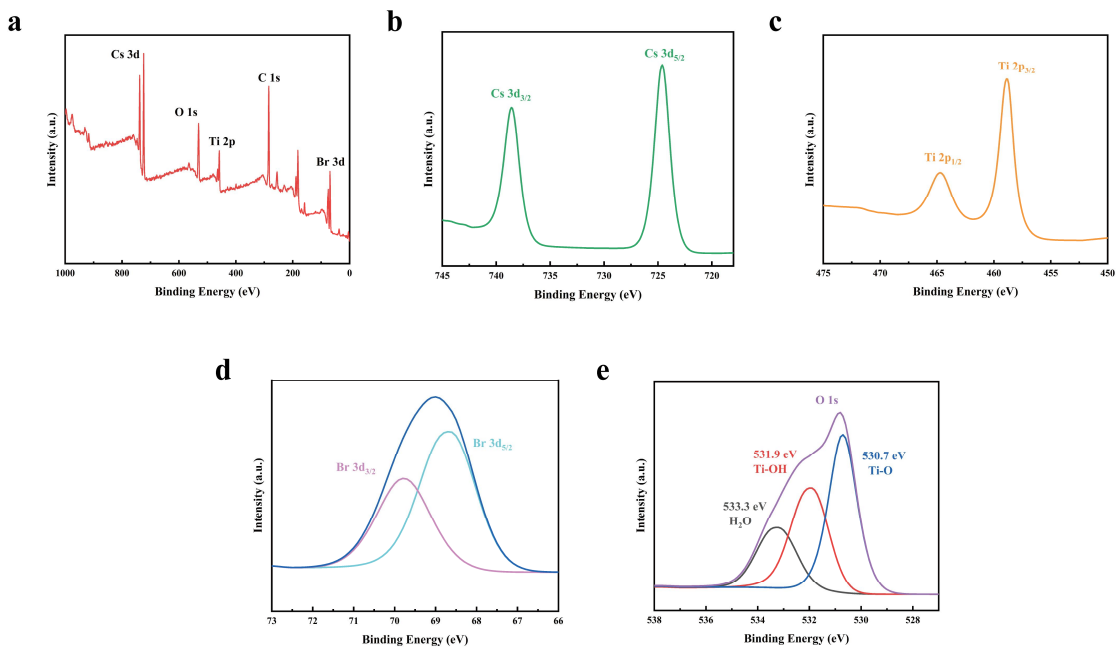

Figure S2 (a) XPS survey spectrum of the Cs_2TiBr_6 powder. The high-resolution XPS spectra of the Cs_2TiBr_6 powder for (b) Cs 3*d*, (c) Ti 2*p*, (c) Br 3*d*, (d) O 1*s*.

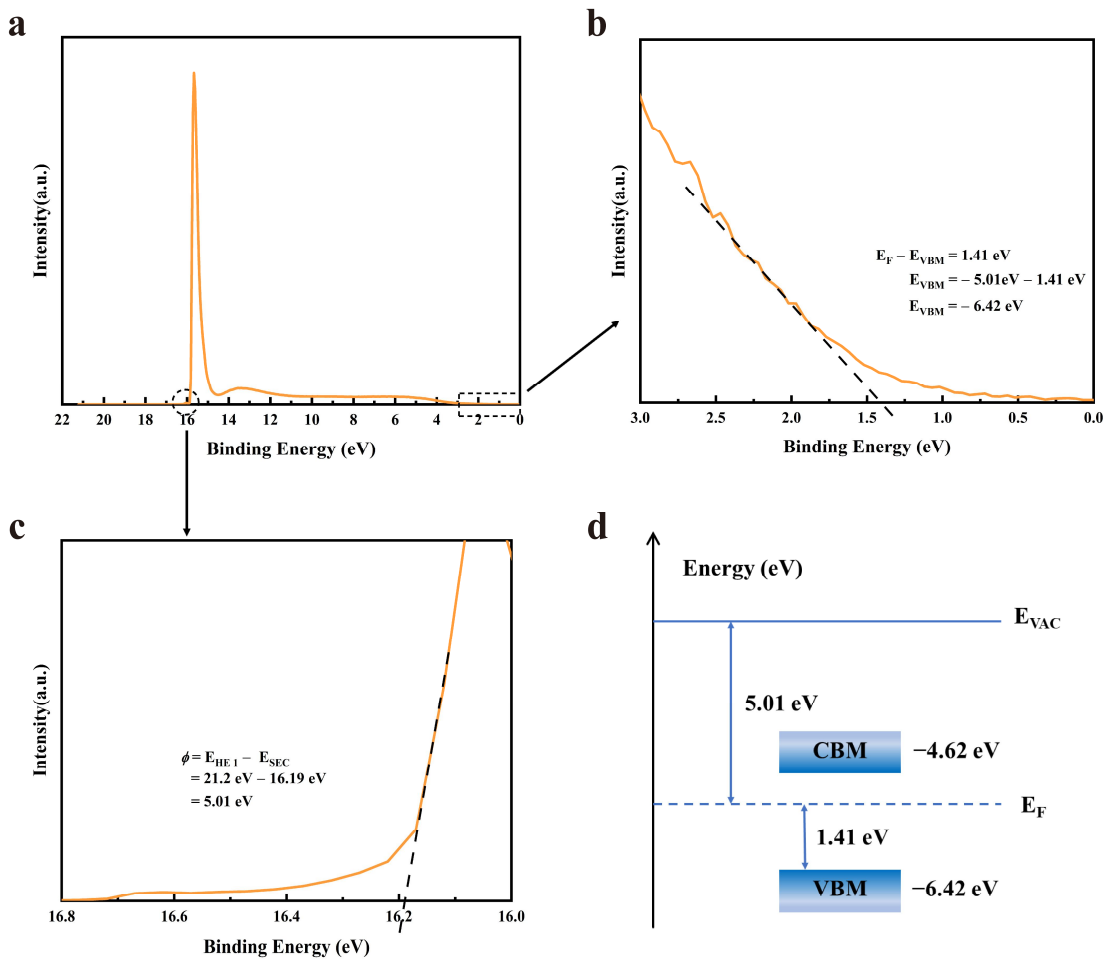

Figure S3 (a-c) UPS characteristics of the Cs_2TiBr_6 powder. (d) Schematic diagram of the band structure for Cs_2TiBr_6 powder.

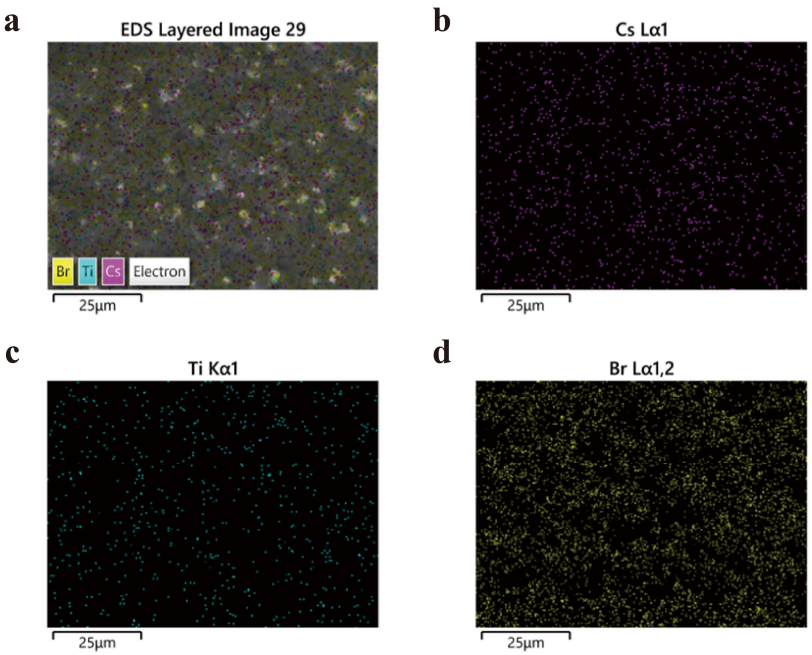

Figure S4 (a-d) EDS element mappings of Cs, Ti and Br in the Cs_2TiBr_6 film.

Table S1 Environmental parameters for stability experiments of Cs_2TiBr_6

Measurement items	Object of measurement	Atmosphere	Temperature	Humidity	Lighting conditions
Ambient air stability	Cs_2TiBr_6 powder	Air	20~25 °C	50~55% RH	Dark
Oxygen stability		Oxygen	20~25 °C	< 0 .1% RH	Dark
Moisture stability		Argon with water vapour	20~25 °C	80% RH	Dark
Thermal stability		Argon	100 °C/200 °C	< 0 .1% RH	Dark
Illumination stability		Argon	30~40 °C	< 0 .1% RH	AM 1.5G
Thermal stability	Cs_2TiBr_6 film	Argon	100 °C/200 °C	< 0.1% RH	Dark
Illumination stability		Argon	30~40 °C	< 0 .1% RH	AM 1.5G

Table S2 Recent studies on the optical properties of Cs_2TiBr_6

Year	Material form	PL emission peak (eV)	PL FWHM (eV)	Stokes shift (eV)	Indirect allowed band gap (eV)	Direct allowed band gap (eV)	Reference
2018	Powder	−	−	−	−	1.78	1
2018	Film	1.8	0.15	0.45	−	1.82	2
2019	Film	1.85	0.25	0.36	1.7	1.94	3
2020	Powder	1.75	0.25	0.5	1.9	2.0	4
2021	Large-grain	−	−	−	1.76	1.86	5
2021	Nanocrystal Suspension	−	−	−	−	1.85 ~ 2.05	6
2021	Nanocrystal Solution	2.1	0.25	0.47	2.0	2.3	7
2022	Powder	1.91	0.29	0.43	1.8	1.95	This work

Reference

1. M.-G. Ju, M. Chen, Y. Zhou, H. F. Garces, J. Dai, L. Ma, N. P. Padture and X. C. Zeng, *ACS Energy Letters*, 2018, **3**, 297-304.
2. M. Chen, M.-G. Ju, A. D. Carl, Y. Zong, R. L. Grimm, J. Gu, X. C. Zeng, Y. Zhou and N. P. J. J. Padture, *Joule*, 2018, **2**, 558-570.
3. D. Kong, D. Cheng, X. Wang, K. Zhang, H. Wang, K. Liu, H. Li, X. Sheng and L. Yin, *Journal of Materials Chemistry C*, 2020, **8**, 1591-1597.
4. J. Euvrard, X. Wang, T. Li, Y. Yan and D. B. Mitzi, *Journal of Materials Chemistry A*, 2020, **8**, 4049-4054.
5. J. L. Mendes, W. Gao, J. L. Martin, A. D. Carl, N. A. Deskins, S. Granados-Focil and R. L. Grimm, *The Journal of Physical Chemistry C*, 2020, **124**, 24289-24297.
6. G. K. Grandhi, A. Matuhina, M. Liu, S. Annurakshita, H. Ali-Löytty, G. Bautista and P. Vivo, *Nanomaterials*, 2021, **11**, 1458.
7. S. M. Liga and G. Konstantatos, *Journal of Materials Chemistry C*, 2021, **9**, 11098-11103.