

Supporting Information

Suppressing intrinsic self-doping of CsPbIBr₂ films for high-performance all-inorganic, carbon-based perovskite solar cells

Zeyang Zhang,^{a,‡} Fengqin He,^{a,c,‡} Weidong Zhu,^{a,*} Dandan Chen,^b Wenming Chai,^a Dazheng Chen,^a He Xi,^a Jincheng Zhang,^a Chunfu Zhang,^{a,*} Yue Hao^a

^aState Key Discipline Laboratory of Wide Band Gap Semiconductor Technology & Shaanxi Joint Key Laboratory of Graphene, School of Microelectronics, Xidian University, Xi'an, Shaanxi 710071, China.

^bCollege of Science, Xi'an Shiyou University, Xi'an, Shaanxi 710065, China.

^cHuanghe Hydropower Solar Industry Technology Co. Ltd., Xi'an, Shanxi 710061, China.

[‡]The authors contribute equally to the work.

*E-mail: wdzhu@xidian.edu.cn, cfzhang@xidian.edu.cn.

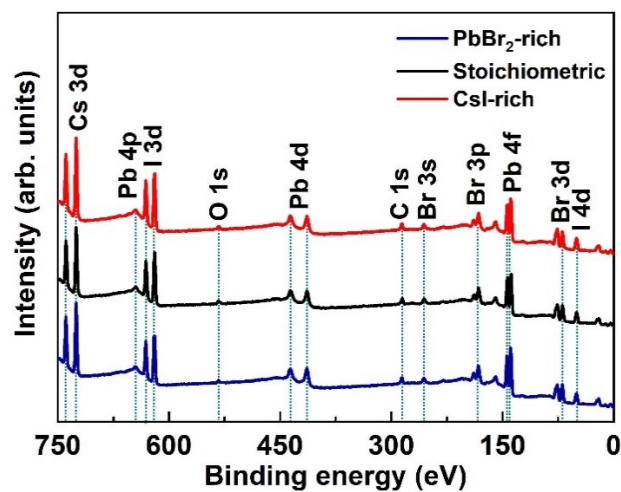


Fig. S1 XPS survey spectra of CsPbIBr₂ films prepared with PbBr₂-rich, stoichiometric, and CsI-rich precursors, respectively.

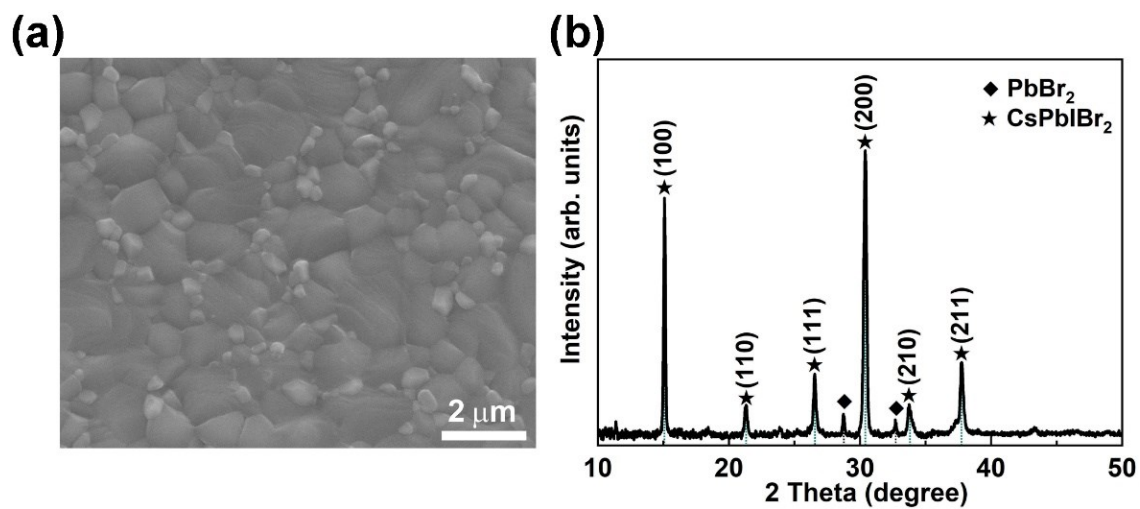


Fig. S2 (a) SEM image and (b) XRD pattern of CsPbIBr₂ film prepared with the precursor with CsI/PbBr₂ stoichiometric ratio of 0.8:1.0.

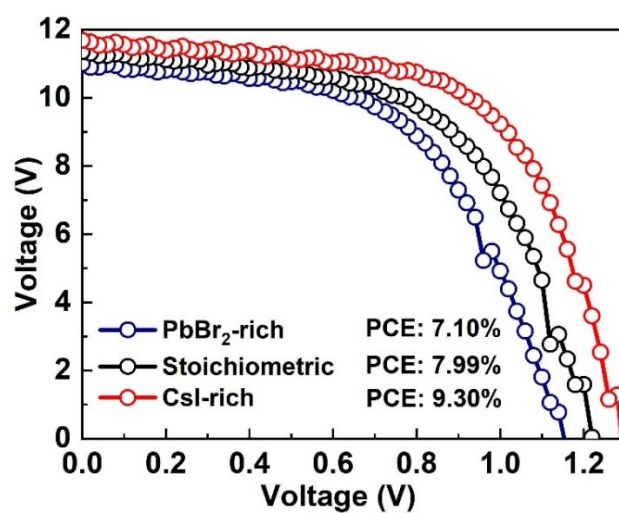


Fig. S3 Light J-V curves recorded under RS voltage scan for the optimized CsPbIBr₂ PSCs based on the typical PbBr₂-rich, stoichiometric, and CsI-rich precursors, respectively.

Table S1. Detailed parameters of (100) and (200) peaks for CsPbIBr₂ films obtained with PbBr₂-rich, stoichiometric, and CsI-rich precursors, respectively.

Samples	Peak of (100) plane			Peak of (200) plane		
	Position (2 θ)	Intensity	FWHM	Position (2 θ)	Intensity	FWHM
PbBr ₂ -rich	15.00°	4012	0.1737°	30.23°	5906	0.2184°
Stoichiometric	15.01°	3622	0.1383°	30.24°	6605	0.1832°
CsI-rich	15.07°	6002	0.1136°	30.35°	8334	0.1784°

Table S2. Summary of PCE and V_{oc} values of CsPbIBr₂-based PSCs reported previously.

Cell configuration	V_{oc} [V]	PCE [%]	Ref.
FTO/c-TiO ₂ /CsPbIBr ₂ /Carbon	1.32	10.48	This work
FTO/TiO ₂ /SmBr ₃ /Sm-doped CsPbIBr ₂ /spiro-OMeTAD/Au	1.14	10.88	[1]
FTO/c-TiO ₂ /CsPbIBr ₂ /Carbon	1.323	10.82	[2]
ITO/SnO ₂ / CsPbIBr ₂ /Spiro-OMeTAD/Ag	1.27	10.81	[3]
FTO/c-TiO ₂ /CsBr/CsPbIBr ₂ /Carbon	1.261	10.71	[4]
FTO/TiO ₂ /CsPb(SO ₃)IBr ₂ /spiro-OMeTAD/Au	1.21	10.55	[5]
FTO/TiO ₂ /CsPb(Ba)IBr ₂ /spiro-OMeTAD/Au	1.19	10.51	[6]
ITO/ZnO-NH ₄ Cl/CsPbIBr ₂ /Spiro-OMeTAD/Ag	1.27	10.16	[7]
ITO/SnO ₂ /CsPbIBr ₂ /YD ₂ -o-C8/spiro-OMeTAD/Ag	1.37	10.13	[8]
ITO/SnO ₂ /S-doped CsPbIBr ₂ /P3HT/Au	1.30	9.78	[9]
FTO/Cs-NiO _x /N749/CsPbIBr ₂ /PC ₆₁ BM/BCP/Ag	1.19	9.49	[10]
FTO/SnO ₂ /TiO ₂ /CsBr/CsPbIBr ₂ /Carbon	1.273	9.31	[11]
FTO/c-TiO ₂ /Li-CsPbIBr ₂ /CuPc/Carbon	1.22	9.25	[12]
FTO/c-TiO ₂ /CsPbIBr ₂ /spiro-OMeTAD/Au	1.20	9.17	[13]
FTO/c-TiO ₂ /CsPbIBr ₂ /Carbon	1.245	9.16	[14]
FTO/c-TiO ₂ /CsPbIBr ₂ /Carbon	1.253	9.12	[15]
FTO/c-TiO ₂ /CsPbIBr ₂ /Carbon	1.258	9.06	[14]
FTO/c-TiO ₂ /CsPbIBr ₂ /Carbon	1.26	9.04	[16]
FTO/c-TiO ₂ /CsPbIBr ₂ /CuPc/Carbon	1.289	8.76	[17]
FTO/c-TiO ₂ /CsPbIBr ₂ /Carbon	1.283	8.60	[18]
ITO/SnO ₂ /CsPbIBr ₂ /spiro-OMeTAD/Ag	1.15	8.54	[19]
FTO/c-TiO ₂ /CsPbIBr ₂ /Carbon	1.05	8.31	[20]
FTO/c-TiO ₂ /m-TiO ₂ /CsPbIBr ₂ /Carbon	1.08	8.25	[21]
FTO/c-TiO ₂ /CsPbIBr ₂ /spiro-OMeTAD/Au	1.227	8.02	[22]
FTO/ZnO/CsPbIBr ₂ /Carbon	1.03	7.60	[23]
ITO/SnO ₂ /C60/CsPbIBr ₂ /spiro-OMeTAD/Au	1.18	7.34	[24]
FTO/TiO ₂ /CsPbIBr ₂ /spiro-OMeTAD/Ag	1.28	7.31	[25]

ITO/Passivated SnO ₂ /CsPbIBr ₂ /Carbon	1.23	7.00	[26]
FTO/c-TiO ₂ /CsPbIBr ₂ /Carbon	1.142	6.55	[27]
FTO/c-TiO ₂ /m-TiO ₂ /CsPbIBr ₂ /spiro-OMeTAD/Au	1.121	6.30	[28]
FTO/c-TiO ₂ /m-TiO ₂ /CsPbIBr ₂ /Carbon	0.96	6.14	[29]
ITO/NiO _x /CsPbIBr ₂ /CeO _x /Ag	1.01	5.60	[30]
FTO/In ₂ S ₃ /CsPbIBr ₂ /Spiro-OMeTAD/Ag	1.09	5.59	[31]
FTO/NiO _x /CsPbIBr ₂ /ZnO/Al	1.01	5.57	[32]
FTO/NiO _x /CsPbIBr ₂ /MoO _x /Au	0.85	5.52	[33]
ITO/SnO ₂ /CsPbIBr ₂ /P3HT/Au	1.07	5.16	[34]
ITO/ZnO/CsPbIBr ₂ /spiro-OMeTAD/Ag	1.04	4.8	[35]
FTO/c-TiO ₂ /CsPbIBr ₂ /Au	0.959	4.70	[36]

References

1. W.S. Subhani, K. Wang, M. Du, X. Wang, S. Liu, *Adv. Energy Mater.*, (2019) 1803785.
2. D. Kim, H.J. Jung, I.J. Park, B.W. Larson, S.P. Dunfield, C. Xiao, J. Kim, J. Tong, P. Boonmongkolras, S.G. Ji, F. Zhang, S.R. Pae, M. Kim, S.B. Kang, V. Dravid, J.J. Berry, J.Y. Kim, K. Zhu, D.H. Kim, B. Shin, *Science*, 368 (2020) 155-160.
3. S. Cao, H. Wang, H. Li, J. Chen, Z. Zang, *Chem. Eng. J.*, (2020) 124903.
4. W. Zhu, Z. Zhang, W. Chai, Q. Zhang, D. Chen, Z. Lin, J. Chang, J. Zhang, C. Zhang, Y. Hao, *ChemSusChem*, 12 (2019) 2318-2325.
5. Y. Wang, K. Wang, W.S. Subhani, C. Zhang, X. Jiang, S. Wang, H. Bao, L. Liu, L. Wan, S.F. Liu, *Small*, (2020) 1907283, DOI: 10.1002/sml.201907283.
6. W.S. Subhani, K. Wang, M. Du, S.F. Liu, *Nano Energy*, 61 (2019) 165-172.
7. H. Wang, S. Cao, B. Yang, H. Li, M. Wang, X. Hu, K. Sun, Z. Zang, *Sol. RRL*, 4 (2020) 1900363.
8. R. Wang, M. Mujahid, Y. Duan, Z.K. Wang, J. Xue, Y. Yang, *Adv. Funct. Mater.*, 29 (2019) 1808843.
9. Z. Wang, A.K. Baranwal, M.A. kamarudin, c.h. Ng, M. Pandey, T. Ma, S. Hayase, *Nano Energy*, 59 (2019) 258-267.
10. S. Yang, L. Wang, L. Gao, J. Cao, Q. Han, F. Yu, Y. Kamata, C. Zhang, M. Fan, G. Wei, *ACS Appl. Mater. Interfaces*, 12 (2020) 13931-13940.
11. W. Zhu, W. Chai, Z. Zhang, D. Chen, J. Chang, S. Liu, J. Zhang, C. Zhang, Y. Hao, *Org. Electron.*, 74 (2019) 103-109.
12. X. Tan, X. Liu, Z. Liu, B. Sun, J. Li, S. Xi, T. Shi, Z. Tang, G. Liao, *Appl. Surf. Sci.*, 499 (2020) 143990.
13. B. Zhang, W. Bi, Y. Wu, C. Chen, H. Li, Z. Song, Q. Dai, L. Xu, H. Song, *ACS Appl. Mater. Interfaces*, 11 (2019) 33868-33878.
14. W. Zhu, Z. Zhang, W. Chai, D. Chen, H. Xi, J. Chang, J. Zhang, C. Zhang, Y. Hao, *ACS Appl. Energy Mater.*, 2 (2019) 5254-5262.

15. W. Zhu, W. Chai, D. Chen, H. Xi, D. Chen, J. Chang, J. Zhang, C. Zhang, Y. Hao, *ACS Appl. Mater. Interfaces*, 12 (2020) 4549-4557.
16. Y. Guo, F. Zhao, Z. Li, J. Tao, D. Zheng, J. Jiang, J. Chu, *Org. Electron.*, 83 (2020) 105731.
17. X. Liu, J. Li, Z. Liu, X. Tan, B. Sun, S. Xi, T. Shi, Z. Tang, G. Liao, *Electrochim. Acta*, 330 (2020) 135266.
18. Q. Zhang, W. Zhu, D. Chen, Z. Zhang, Z. Lin, J. Chang, J. Zhang, C. Zhang, Y. Hao, *ACS Appl. Mater. Interfaces*, 11 (2018) 2997-3005.
19. Y. Jiang, J. Yuan, Y. Ni, J. Yang, Y. Wang, T. Jiu, M. Yuan, J. Chen, *Joule*, 2 (2018) 1356-1368.
20. C. Wang, J. Zhang, J. Duan, L. Gong, J. Wu, L. Jiang, C. Zhou, H. Xie, Y. Gao, H. He, *Mater. Sci. Semicond. Process.*, 108 (2020) 104870.
21. J. Liang, P. Zhao, C. Wang, Y. Wang, Y. Hu, G. Zhu, L. Ma, J. Liu, Z. Jin, *J. Am. Chem. Soc.*, 139 (2017) 14009-14012.
22. W. Li, M.U. Rothmann, A. Liu, Z. Wang, Y. Zhang, A.R. Pascoe, J. Lu, L. Jiang, Y. Chen, F. Huang, *Adv. Energy Mater.*, 7 (2017) 1700946.
23. C. Wang, J. Zhang, L. Jiang, L. Gong, H. Xie, Y. Gao, H. He, Z. Fang, J. Fan, Z. Chao, *J. Alloys and Compd.*, 817 (2020) 152768.
24. N. Li, Z. Zhu, J. Li, A.K.Y. Jen, L. Wang, *Adv. Energy Mater.*, 8 (2018) 1800525.
25. J. Lu, S.-C. Chen, Q. Zheng, *ACS Appl. Energy Mater.*, 1 (2018) 5872-5878.
26. Z. Guo, S. Teo, Z. Xu, C. Zhang, Y. Kamata, S. Hayase, T. Ma, *J. Mater. Chem. A*, 7 (2019) 1227-1232.
27. W. Zhu, Q. Zhang, C. Zhang, Z. Zhang, D. Chen, Z. Lin, J. Chang, J. Zhang, Y. Hao, *ACS Appl. Energy Mater.*, 1 (2018) 4991-4997.
28. C.F.J. Lau, X. Deng, Q. Ma, J. Zheng, J.S. Yun, M.A. Green, S. Huang, A.W. Ho-Baillie, *ACS Energy Lett.*, 1 (2016) 573-577.
29. J. Liang, Z. Liu, L. Qiu, Z. Hawash, L. Meng, Z. Wu, Y. Jiang, L.K. Ono, Y. Qi, *Adv. Energy Mater.*, 8 (2018) 1800504.
30. J. Yang, Q. Zhang, J. Xu, H. Liu, R. Qin, H. Zhai, S. Chen, M. Yuan, *Nanomaterials*, 9 (2019) 1666.
31. B. Yang, M. Wang, X. Hu, T. Zhou, Z. Zang, *Nano Energy*, 57 (2019) 718-727.
32. J. Lin, M. Lai, L. Dou, C.S. Kley, H. Chen, F. Peng, J. Sun, D. Lu, S.A. Hawks, C. Xie, *Nat. Mater.*, 17 (2018) 261.
33. C. Liu, W. Li, J. Chen, J. Fan, Y. Mai, R.E. Schropp, *Nano Energy*, 41 (2017) 75-83.
34. Z. Wang, A. Baranwal, *Nano Energy*, 59 (2019) 258-267.
35. M. Aamir, T. Adhikari, M. Sher, N. Revaprasadu, W. Khalid, J. Akhtar, J.-M. Nunzi, *New J. Chem.*, 42 (2018) 14104-14110.
36. Q. Ma, S. Huang, X. Wen, M.A. Green, A.W. Ho-Baillie, *Adv. Energy Mater.*, 6 (2016) 1502202.