

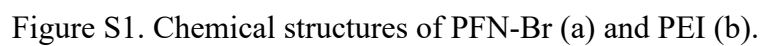
Supporting Information for

Management of interfacial energy band alignment in wide-bandgap perovskite solar cells for performance improvement

Zhihai Liu,^{a,*} Lei Wang,^b Jiqu Han,^a Hao Zhao,^a Ren Sheng^a and Ping Chen^{a,**}

^aSchool of Physics and Electronic Information, Yantai University, Yantai 264005, China, *Emails:*
zhliu@ytu.edu.cn and chenping@ytu.edu.cn

^bSchool of Artificial Intelligence, Beijing Technology and Business University, Beijing, 100048, China



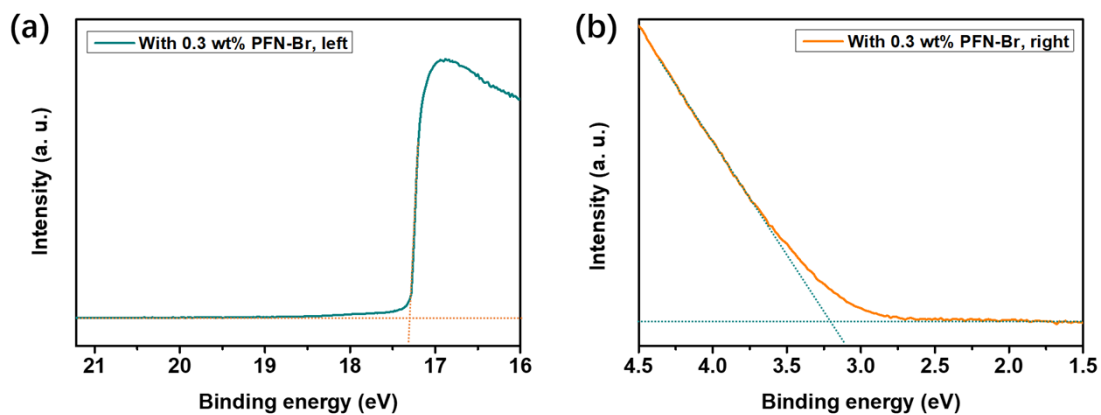


Figure S3. Left (d) and right (e) regions of the UPS spectra for the SnO_2 film with 0.3 wt% PFN-Br.

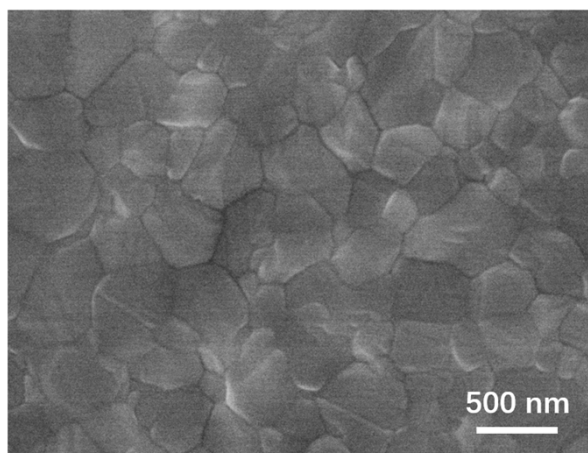


Figure S4. SEM image of the prepared $\text{Cs}_{0.15}\text{FA}_{0.79}\text{MA}_{0.06}\text{Pb}(\text{I}_{0.7}\text{Br}_{0.3})_3$ perovskite film.

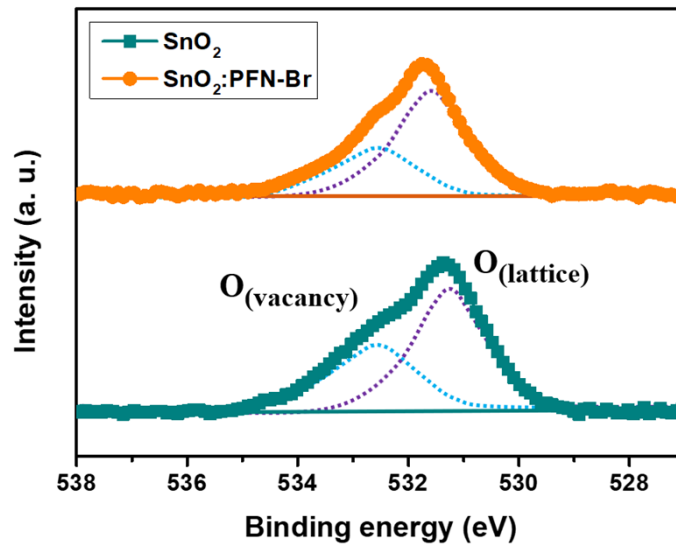


Figure S5. XPS spectra of O 1s orbital for pristine SnO_2 and PFN-Br incorporated SnO_2 films.

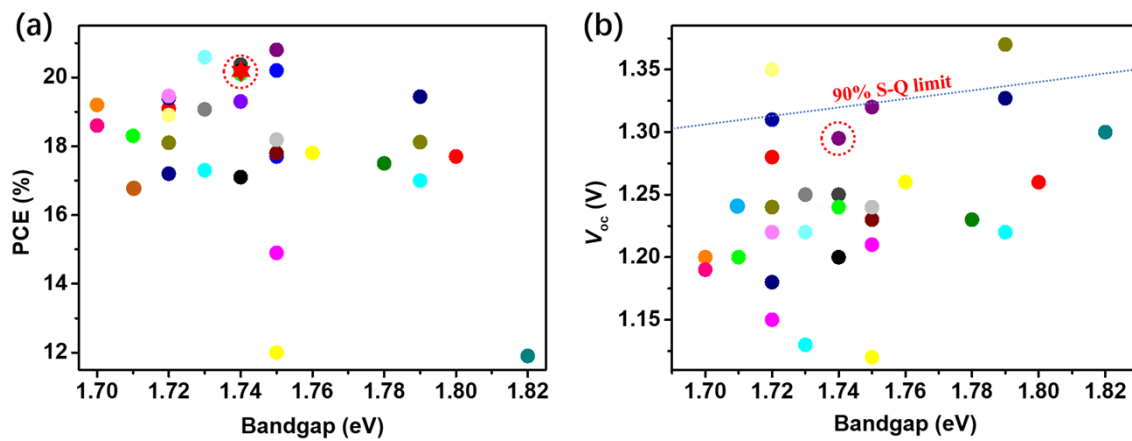


Figure S6. Relationships of (a) PCE and perovskite bandgap; (b) V_{oc} and perovskite bandgap.

Table S1. Device parameters for recently reported wide-bandgap PSCs.

No.	V_{oc} (V)	PCE (%)	Bandgap (eV)	Reference
1	1.20	17.1	1.74	[1]
2	1.28	19.1	1.72	[2]
3	1.20	18.3	1.71	[3]
4	1.23	17.7	1.75	[4]
5	1.13	17.3	1.73	[5]
6	1.15	17.2	1.72	[6]
7	1.12	12.0	1.75	[7]
8	1.24	18.1	1.72	[8]
9	1.18	17.2	1.72	[9]
10	1.28	20.2	1.74	This work
11	1.23	17.8	1.75	[10]
12	1.23	17.5	1.78	[11]
13	1.30	11.9	1.82	[12]
14	1.31	19.4	1.72	[13]
15	1.20	19.2	1.70	[14]
16	1.25	19.3	1.74	[15]
17	1.19	18.6	1.70	[16]
18	1.24	16.74	1.71	[17]
19	1.24	18.19	1.75	[18]
20	1.25	19.07	1.73	[19]
21	1.35	18.9	1.72	[20]
22	1.22	20.59	1.73	[21]
23	1.22	19.46	1.72	[22]
24	1.25	20.37	1.74	[23]
25	1.25	20.2	1.74	[24]
26	1.26	17.7	1.80	[25]
27	1.24	20.1	1.74	[26]
28	1.21	20.2	1.75	[27]
29	1.22	17.0	1.79	[28]
30	1.21	14.9	1.75	[29]
31	1.26	17.8	1.76	[30]
32	1.37	18.12	1.79	[31]
33	1.32	20.8	1.75	[32]
34	1.327	19.44	1.79	[33]

Reference

- [1] D. P. Mcmeekin, G. Sadoughi, W. Rehman, G. E. Eperon, M. Saliba, M. T. Hörantner, A. Haghighirad, N. Sakai, L. Korte, B. Rech, M. B. Johnston, L. M. Herz, H. J. Snaith. *Science*, **2016**, 351, 151.
- [2] T. Duong, H. Pham, Y. Yin, J. Peng, M. A. Mahmud, Y. Wu, H. Shen, J. Zheng, T. Tran-Phu, T. Lu, L. Li, A. Kumar, G. G. Andersson, A. Ho-Baillie, Y. Liu, T. White, K. Weber, K. Catchpole. *J. Mater. Chem. A*, **2021**, 9, 18454.
- [3] Y. Lin, B. Chen, F. Zhao, X. Zheng, Y. Deng, Y. Shao, Y. Fang, Y. Bai, C. Wang, J. Huang. *Adv. Mater.*, **2017**, 29, 1700607.
- [4] Y. Yu, C. Wang, C. R. Grice, N. Shrestha, D. Zhao, W. Liao, L. Guan, R. A. Awni, W. Meng, A. J. Cimaroli, K. Zhu, R. J. Ellingson, Y. Yan. *ACS Energy Lett.*, **2017**, 2, 1177.
- [5] T. Duong, Y. Wu, H. Shen, J. Peng, X. Fu, D. Jacobs, E.-C. Wang, T. C. Kho, K. C. Fong, M. Stocks, E. Franklin, A. Blakers, N. Zin, K. McIntosh, W. Li, Y.-B. Cheng, T. P. White, K. Weber, K. Catchpole. *Adv. Energy Mater.*, **2017**, 7, 1700228.
- [6] Z. Wang, Q. Lin, F. P. Chmiel, N. Sakai, L. M. Herz, H. J. Snaith. *Nat. Energy*, **2017**, 2, 17135.
- [7] R. J. Stoddard, F. T. Eickemeyer, J. K. Katahara, H. W. Hillhouse, *J. Phys. Chem. Lett.*, **2017**, 8, 3289.
- [8] Y. Zhou, F. Wang, Y. Cao, J.-P. Wang, H.-H. Fang, M. A. Loi, N. Zhao, C.-P. Wong. *Adv. Energy Mater.*, **2017**, 7, 1701048.
- [9] Z. Wang, Q. Lin, F. P. Chmiel, N. Sakai, L. M. Herz, H. J. Snaith. *Nat. Energy*, **2017**, 2, 17135.
- [10] J. Kim, M. I. Saidaminov, H. Tan, Y. Zhao, Y. Kim, J. Choi, J. W. Jo, J. Fan, R. Quintero-Bermudez, Z. Yang, L. N. Quan, M. Wei, O. Voznyy, E. H. Sargent, *Adv. Mater.*, **2018**, 30, 1706275.
- [11] M. Abdi-Jalebi, Z. Andaji-Garmaroudi, S. Cacovich, C. Stavrakas, B. Philippe, J. M. Richter, M. Alsari, E. P. Booker, E. M. Hutter, A. J. Pearson, S. Lilliu, T. J. Savenije, H. Rensmo, G. Divitini, C. Ducati, R. H. Friend, S. D. Stranks. *Nature*, **2018**, 555, 497.
- [12] A. Rajagopal, R. J. Stoddard, S. B. Jo, H. W. Hillhouse, A. K. Y. Jen, *Nano Lett.*, **2018**, 18, 3985.
- [13] S. Gharibzadeh, B. Abdollahi Nejand, M. Jakoby, T. Abzieher, D. Hauschild, S. Moghadamzadeh, J. A. Schwenzer, P. Brenner, R. Schmager, A. A. Haghighirad, L. Weinhardt, U. Lemmer, B. S. Richards, I. A. Howard, U. W. Paetzold, *Adv. Energy Mater.*, **2019**, 9, 1803699.

- [14] A. F. Palmstrom, G. E. Eperon, T. Leijtens, R. Prasanna, S. N. Habisreutinger, W. Nemeth, E. A. Gaulding, S. P. Dunfield, M. Reese, S. Nanayakkara, T. Moot, J. Werner, J. Liu, B. To, S. T. Christensen, M. D. McGehee, M. F. a. M. Van Hest, J. M. Luther, J. J. Berry, D. T. Moore. *Joule*, **2019**, 3, 2193.
- [15] H. Tan, F. Che, M. Wei, Y. Zhao, M. I. Saidaminov, P. Todorović, D. Broberg, G. Walters, F. Tan, T. Zhuang, B. Sun, Z. Liang, H. Yuan, E. Fron, J. Kim, Z. Yang, O. Voznyy, M. Asta, E. H. Sargent. *Nat. Commun.*, **2018**, 9, 3100.
- [16] B. Chen, Z. Yu, K. Liu, X. Zheng, Y. Liu, J. Shi, D. Spronk, P. N. Rudd, Z. Holman, J. Huang. *Joule*, **2019**, 3, 177.
- [17] D. B. Khadka, Y. Shirai, M. Yanagida, T. Noda, K. Miyano. *ACS Appl. Mater. Interfaces*, **2018**, 10, 22074.
- [18] C. Chen, Z. Song, C. Xiao, D. Zhao, N. Shrestha, C. Li, G. Yang, F. Yao, X. Zheng, R. J. Ellingson, C.-S. Jiang, M. Al-Jassim, K. Zhu, G. Fang, Y. Yan. *Nano Energy*, **2019**, 61, 141.
- [19] C. Chen, Z. Song, C. Xiao, R. A. Awni, C. Yao, N. Shrestha, C. Li, S. S. Bista, Y. Zhang, L. Chen, R. J. Ellingson, C.-S. Jiang, M. Al-Jassim, G. Fang, Y. Yan. *ACS Energy Lett.*, **2020**, 5, 2560.
- [20] Z. Liu, J. Siekmann, B. Klingebiel, U. Rau, T. Kirchartz, *Adv. Energy Mater.*, **2021**, 11, 2003386.
- [21] L. Tao, X. Du, J. Hu, S. Wang, C. Lin, Q. Wei, Y. Xia, G. Xing, Y. Chen. *Sci. China Chem.*, **2022**, 65, 1650.
- [22] C. Tian, X. Gao, J. Li, J. Pan, G. Yu, B. Huang, Y. Wen, H. Zhu, T. Bu, Y.-B. Cheng, F. Huang, *Solar RRL*, **2022**, 6, 2200134.
- [23] L. Liu, Y. Yang, M. Du, Y. Cao, X. Ren, L. Zhang, H. Wang, S. Zhao, K. Wang, S. Liu. *Adv. Energy Mater.*, **2023**, 13, 2202802.
- [24] Z. Liu, L. Wang, X. Xie, C. Xu, C. Zhang, P. Chen, *J. Mater. Chem. C*, **2023**, 11, 15898.
- [25] J. Wen, Y. Zhao, Z. Liu, H. Gao, R. Lin, S. Wan, C. Ji, K. Xiao, Y. Gao, Y. Tian, J. Xie, C. J. Brabec, H. Tan. *Adv. Mater.*, **2022**, 34, 2110356.
- [26] Z. Liu, L. Wang, X. Liu, X. Xie, P. Chen, *Nanoscale*, **2024**, 16, 7670.
- [27] M. A. Mahmud, J. Zheng, S. Tang, G. Wang, J. Bing, A. D. Bui, J. Qu, L. Yang, C. Liao, H. Chen, S. P. Bremner, H. T. Nguyen, J. Caine, A. W. Y. Ho-Baillie. *Adv. Energy Mater.*, **2022**, 22, 2201672.
- [28] R. D. J. Oliver, P. Caprioglio, F. Peña-Camargo, L. R. V. Buizza, F. Zu, A. J. Ramadan, S. G. Motti, S. Mahesh, M. M. McCarthy, J. H. Warby, Y.-H. Lin, N. Koch, S. Albrecht, L. M. Herz, M. B. Johnston, D. Neher, M. Stolterfoht, H. J. Snaith. *Energy Environ. Sci.*, **2022**, 15, 714.

- [29] M. Hu, C. Bi, Y. Yuan, Y. Bai, J. Huang, *Adv. Sci.*, **2016**, 3, 1500301.
- [30] Y.-H. Chiang, K. Frohna, H. Salway, A. Abfalterer, L. Pan, B. Roose, M. Anaya, S. D. Stranks. *ACS Energy Lett.*, **2023**, 8, 2728.
- [31] Z. Wei, Q. Zhou, X. Niu, S. Liu, Z. Dong, H. Liang, J. Chen, Z. Shi, X. Wang, Z. Jia, X. Guo, R. Guo, X. Meng, Y.-D. Wang, N. Li, Z. Xu, Z. Li, A. G. Aberle, X. Yin, Y. Hou, *Energy Environ. Sci.*, **2025**, 18, 1847.
- [32] R. Wang, X. Liu, S. Yan, N. Meng, X. Zhao, Y. Chen, H. Li, S. M. H. Qaid, S. Yang, M. Yuan, T. He, *Nat. Commun.*, **2024**, 15, 8899.
- [33] X. Meng, X. Liu, Q. Zhou, Z. Liu, W. Chen, *Nano Energy*, **2024**, 128, 109984.