Electronic Supplementary Material (ESI) for Nanoscale. This journal is © The Royal Society of Chemistry 2019

Electronic Supplementary Information

Band engineering at the interface of all-inorganic CsPbI₂Br solar cells

Jing Zhuang,^{a,b} Yuanzhi Wei,^{a,b} Yigang Luan,^{a,b} Ningli Chen,^{a,b} Peng Mao,^{*a,b} Shaokui Cao^{*c} and Jizheng Wang^{*a,b}

 ^a Beijing National Laboratory for Molecular Sciences, CAS Key Laboratory of Organic Solids, Institute of Chemistry, Chinese Academy of Sciences, Beijing 100190, China
^b University of Chinese Academy of Sciences, Beijing 100049, China
E-mail: maopengpku@iccas.ac.cn; jizheng@iccas.ac.cn
^c School of Materials Science and Engineering, Zhengzhou University, Zhengzhou 450001, PR China
*Corresponding author.
E-mail address: jizheng@iccas.ac.cn(J. Wang), caoshaokui@zzu.edu.cn(S. Cao), maopengpku@iccas.ac.cn(P. Mao)



Fig. S1. Fundamental characteristics of BrBeAI: (a) the molecular structure, (b)

thermogravimetric Analysis (TGA) pattern.



Fig. S2. Atomic force microscopy (AFM) images of the BrBeAI-CsPbI₂Br thin films.

(a) pristine perovskite, (b) BrBeAI-1, (c) BrBeAI-2, (d) BrBeAI-4.



Fig. S3. Morphologies and structure characteristics of CsPbI₂Br thin films treated with different BrBeAI contents: (a) and (b) top-surface SEM images, (c) N 1s

core-level spectra and (d) XRD patterns.



Fig. S4. FTIR patterns of BrBeAI, pristine perovskite, and BrBeAI-4 thin films.



Fig. S5. XPS spectra for the pristine perovskite, BrBeAI-1, BrBeAI-2 and BrBeAI-4

thin films.



Fig. S6. (a) Cs 3d and (b) Pb 4f core-level spectra for the pristine perovskite,

BrBeAI-1, BrBeAI-2 and BrBeAI-4 thin films.



Fig. S7. PL spectra for pristine perovskite, BrBeAI-1, BrBeAI-2 and BrBeAI-4 thin



films.

Fig. S8. TRPL of pristine perovskite, BrBeAI-1, BrBeAI-2 and BrBeAI-4 thin films.



Fig. S9. The water contact angle characterization for pristine perovskite and

BrBeAI-2 thin films.



Fig. S10. XRD patterns of BrBeAI.



Fig. S11. J-V characteristics of BrBeAI-2 based PSC under both the reverse and

forward scan directions.



Fig. S12. Electrical stability measured as a function of time for the BrBeAI-2 based PSC at a voltage of 0 V under 1 sun illumination in a N_2 glovebox. After 30 minutes,

this device retains 87% of its initial $J_{\rm sc}$.



Fig. S13. PCE decay of the pristine and BrBeAI-2 based PSCs as a function of

storage time in a dark and dry box with 20% RH at RT.



Fig. S14. Thermal stability measured for the pristine and BrBeAI-2 based PSCs at 60 $^{\circ}$ C in a N₂ glovebox. After 100 h, the BrBeAI-2 based device maintains 88% of its initial

PCE. Moreover, the pristine device maintains 85% of its initial PCE.