

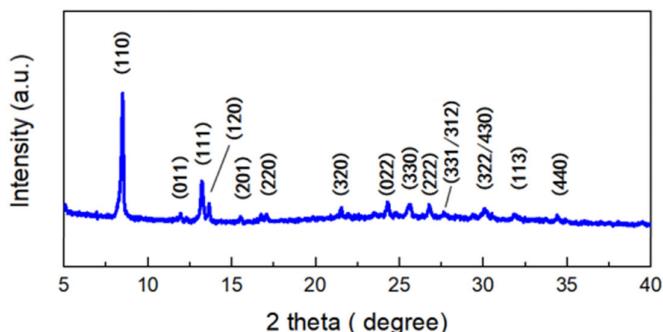
## Supplementary Materials

# Effect of Polarization on Performance of Inverted Electron Transport Layer-Free Solar Cells Based on Molecular Ferroelectric Hexane-1,6-Diammonium Pentaiodobismuth

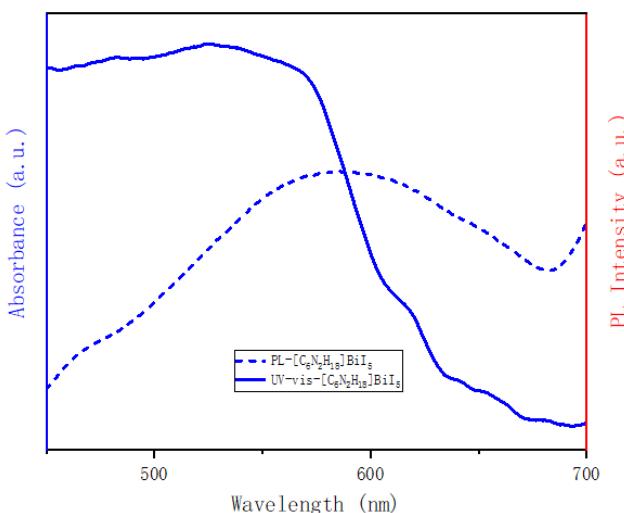
Xiaolan Wang, Xiaoping Zou \*, Jialin Zhu \*, Chunqian Zhang, Jin Cheng, Junming Li, Zixiao Zhou, Yifei Wang, Xiaotong Li, Keke Song and Baokai Ren

Beijing Advanced Innovation Center for Materials Genome Engineering, Beijing Key Laboratory for Sensor, Beijing Key Laboratory for Optoelectronic Measurement Technology, MOE Key Laboratory for Modern Measurement and Control Technology, School of Automation, Beijing Information Science and Technology University, Jianxiangqiao Campus, Beijing 100101, China; wangxl1105@163.com (X.W.); chunqiancool@163.com (C.Z.); chengjin@bistu.edu.cn (J.C.); 18049217206@163.com (Z.Z.); yifewang2020@126.com (Y.W.); xiaotong252240@163.com (X.L.); brenbk2021@163.com (B.R.); songmengke163@163.com (K.S.); li@bistu.edu.cn (J.L.).

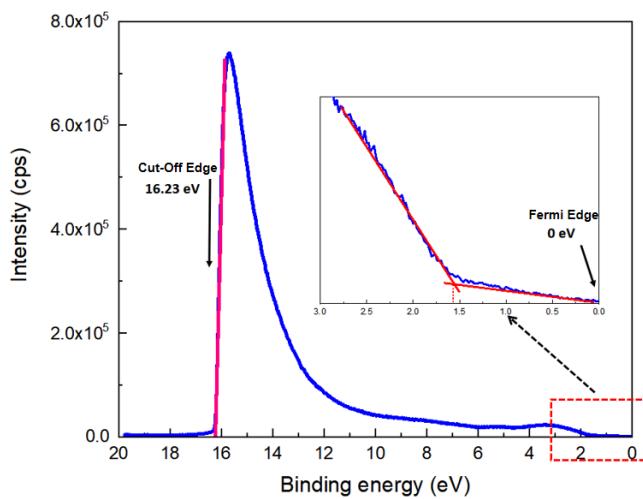
\* Correspondence: xpzou2014@163.com (X.Z.); jlzhu@bistu.edu.cn (J.Z.); Tel.: +86-1364-105-6404 (X.Z.)



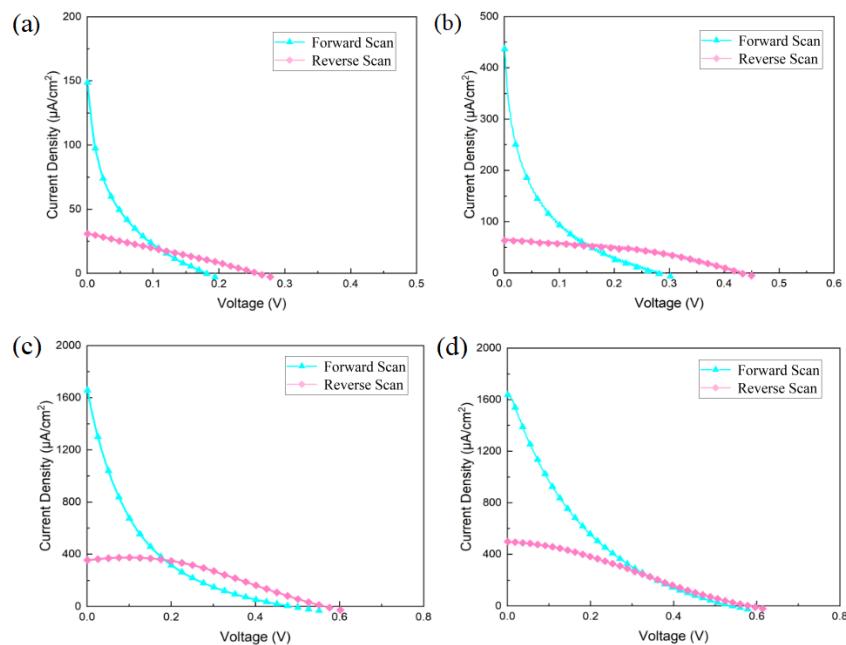
**Figure S1.** X-ray diffraction spectra of organic-inorganic hybrid ferroelectric materials.



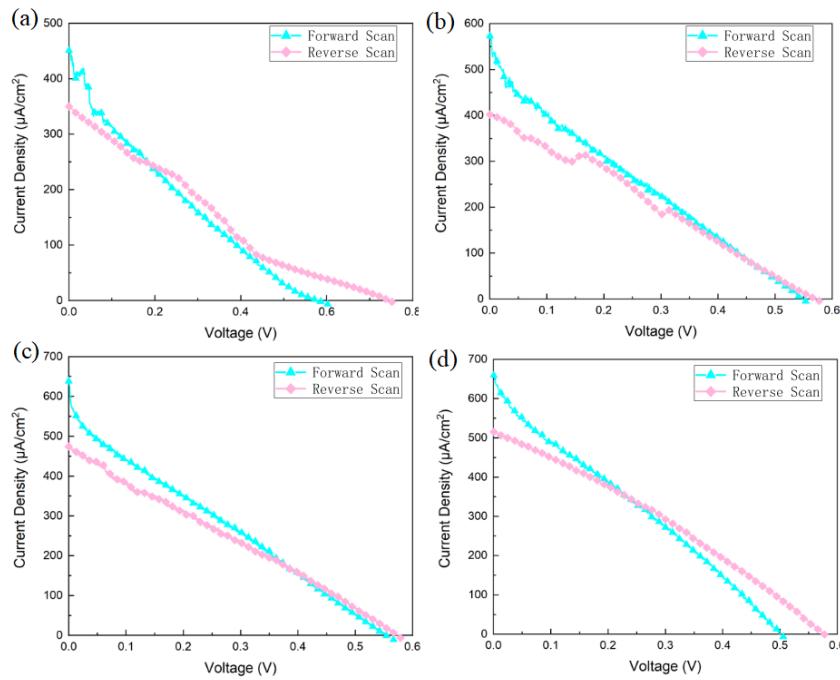
**Figure S2.** Ultraviolet-visible light (UV-vis) absorption spectra and photoemission spectra (PL) of organic-inorganic hybrid ferroelectric films.



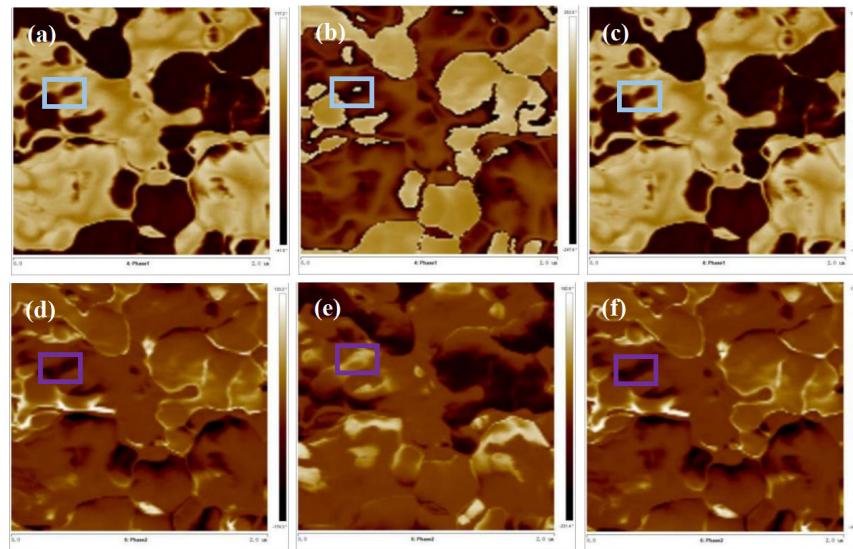
**Figure S3.** Ultraviolet Photoelectron Spectroscopy (UPS) of Organic-inorganic Hybrid Ferroelectric Material HDA-BiI<sub>3</sub>.



**Figure S4.** J-V curves of ITO/NiO<sub>x</sub>/HDA-BiI<sub>3</sub>/PCBM/Ag structure devices after different constant voltage polarization. (a) 0.6V, (b) 0.8V, (c) 1.0V, (d) 1.2V.



**Figure S5.** J-V curves of the optimized device after different voltage polarization. (a) 0.6V, (b) 0.8V,(c) 1.0V, (d) 1.2V.



**Figure S6.** The vertical PFM phase angles of ferroelectric films are (a) -10 V, (b) 10 V, (c) -10 V and the horizontal PFM phase angles are (d) -10 V, (e) 10 V, (f) -10 V.