

Supporting Information

Multiple Strategies to Greatly Enhance the Photovoltaic Characteristics of BiFeO₃-based Films

Zehao Sun,¹ Jie Wei,^{1,*} Shigeng Song,² Minchuan Xiahou,¹ Ao Cao,¹ Junlong Zhang,¹ Youxin Yuanfeng,¹ Guogang Chen,¹ Yongqiang Chen³

¹ *Electronic Materials Research Laboratory, Key Laboratory of Ministry of Education & Shaanxi Engineering Research Center of Advanced Energy Materials and Devices, School of Electronic Science and Engineering, Xi'an Jiaotong University, Xi'an 710049, P. R. China*

² *Institute of Thin Films, Sensors and Imaging, University of the West of Scotland, SUPA Paisley PA1 2BE, Scotland, UK*

³ *School of Material Science and Engineering, Zhengzhou University, Henan 450001, China*

***Corresponding Author:**

Jie Wei, E-mail address: weij2008@xjtu.edu.cn ; jiewei2013wj@gmail.com

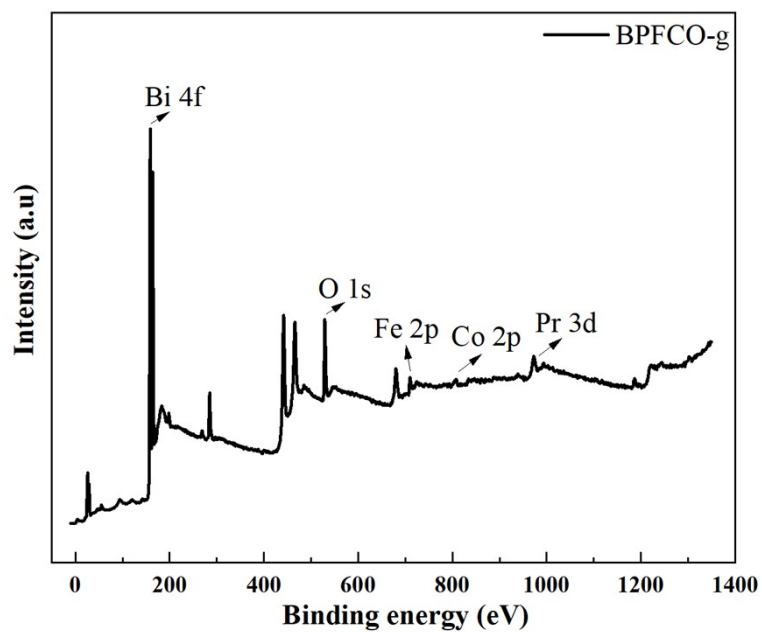


Figure S1. XPS survey spectra analysis of gradient doped sample BPFfCO-g

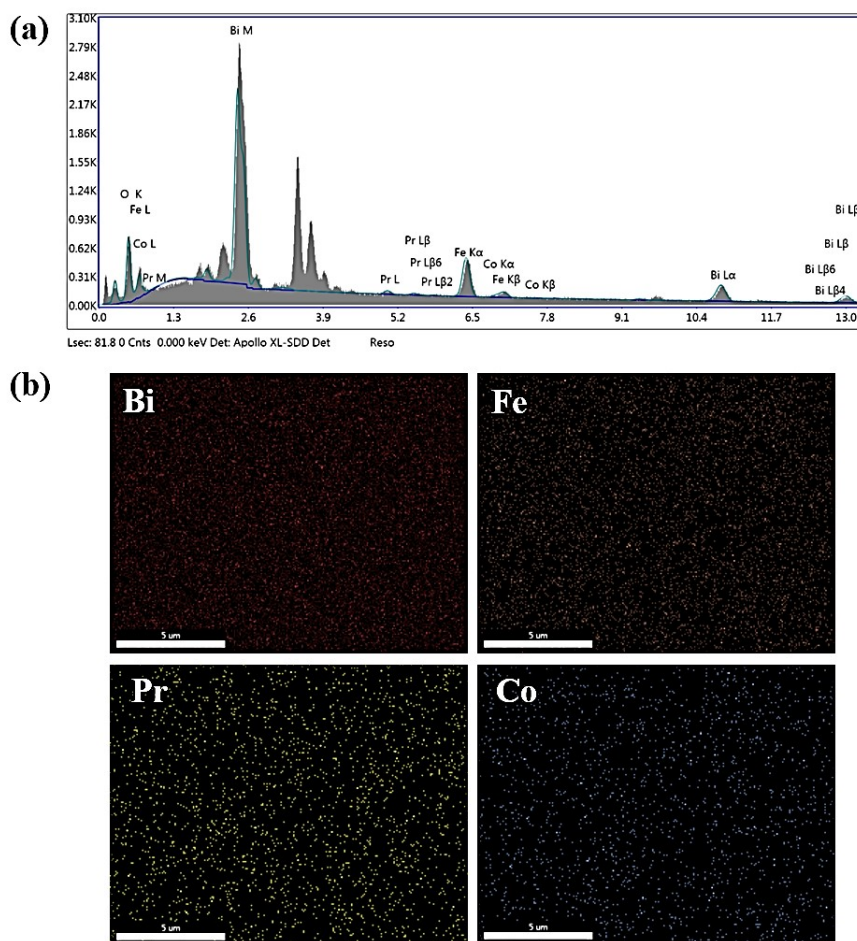


Figure S2. (a) EDS spectrum and (b) element Mapping analysis of gradient doped sample BPFfCO-g

As shown in Fig. S1, all the element peaks of Bi4f, O1s, Fe2p, Co2p and Pr3d can be clearly observed in the sample of BPF_{CO}-g. As shown in Fig. S2, both EDS spectrum and element mapping analysis clearly confirm that the elements of Co and Pr are indeed present in the sample of BPF_{CO}-g.

All in all, XPS survey spectra and EDS mapping analysis clearly confirm that the elements of Co and Pr are indeed present in the doped samples.

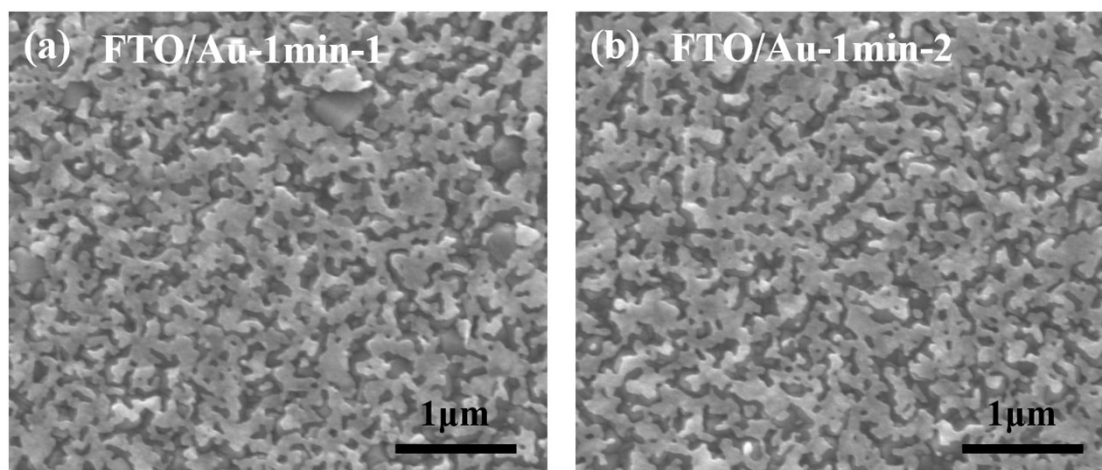


Figure S3. SEM images of (a) first sample of FTO/Au-1mins and (b) second sample of FTO/Au-1mins.

As shown in Fig. S3, SEM images show that the microscopic morphologies of the two samples “FTO/Au-1mins” were not significantly different, which suggests that “the Au on the surface of each sample is the almost same, because it undergoes the same procedure”.

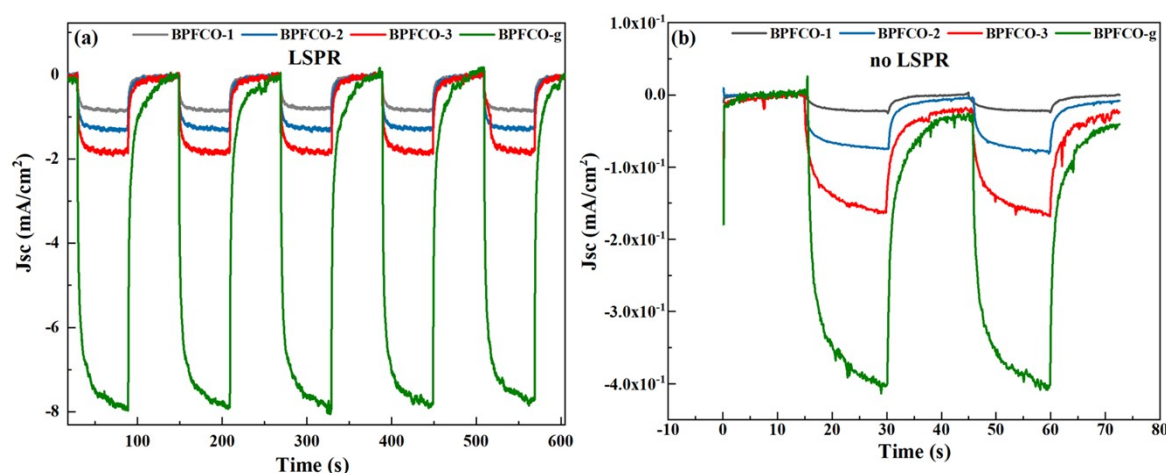


Figure S4. Short-circuit current density of four samples (a) with LSPR effect and (b) without LSPR effect

As shown in Figure S4 and Table 4, the short-circuit current density (J_{sc}) of four samples (BPFCO-1, BPFCO-2, BPFCO-3, BPFCO-g) with and without LSPR effect is compared. Obviously, J_{sc} of four samples with LSPR effect is much larger than that without Au nanoparticles, which is evidence to support the LSPR effect of the Au nanoparticles.

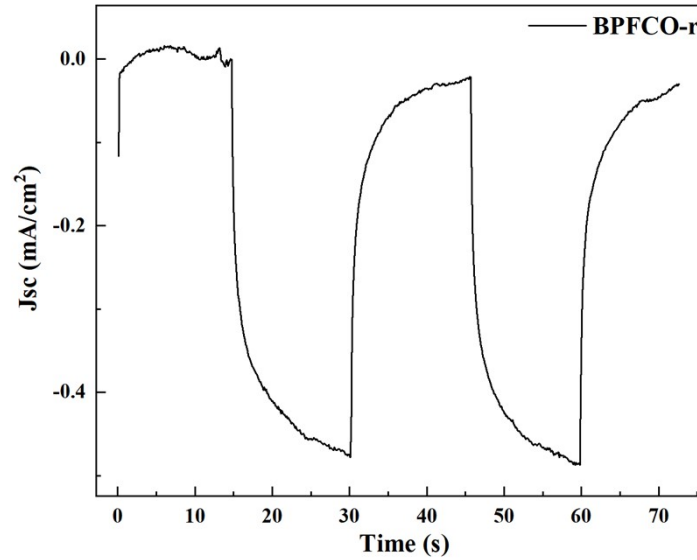


Figure S5. Short-circuit current density of reverse gradient doped sample BPFCO-r

Table S1 Photovoltaic parameters of BPFCO-x (x=1,2,3,g,r) films

	BPFCO-1	BPFCO-2	BPFCO-3	BPFCO-g	BPFCO-r
$J_{sc}(\text{Au-NPs})$	0.8 mA/cm ²	1.3 mA/cm ²	1.8 mA/cm ²	8 mA/cm ²	0.4 mA/cm ²

The reverse gradient doped sample of BPFCO-r (BPFCO-3/BPFCO-2/BPFCO-1/Au-NPs/FTO) was also constructed. In this sample, the two built-in electric field E_{bi-gv} and E_{flex} have the opposite direction. In this way, the two electric fields are cancelling each other out, rather than acting in synergy. Consequently, the short-circuit current density should be very low. As shown in Fig. S5 and Table S1, its short-circuit current density was 0.4 mA/cm², which is even lower than that of the conventional doped sample BPFCO-1. The reason is that the reverse gradient doping causes the two built-in electric

field to cancel out each other, weakening the separation of photo generated carriers, and thus reducing its short-circuit current density.

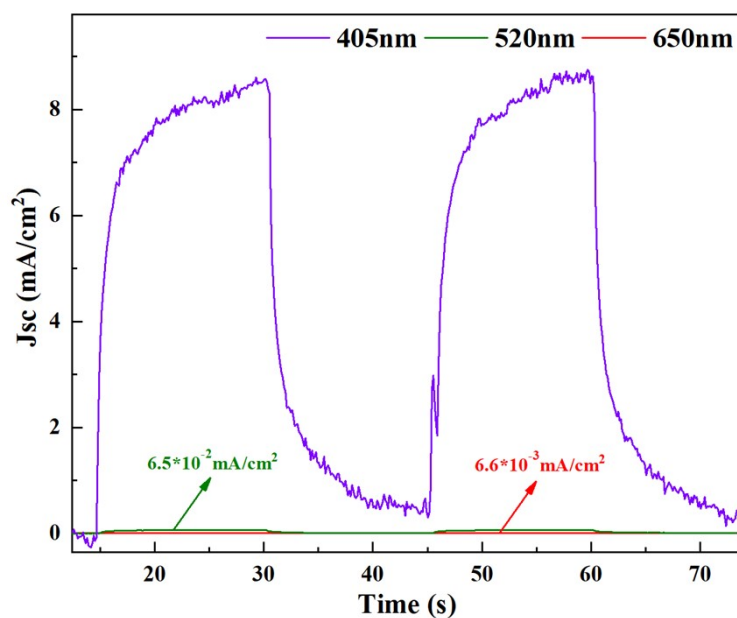


Figure S6. *Jsc-T curves of BPFCO-g under three different wavelengths*

Table S3 *Short circuit current densities of BPFCO-g under three different wavelengths*

Wavelength (nm)	405	520	650
Jsc (mA/cm ²)	8	6.5×10^{-2}	6.6×10^{-3}

Figure S6 shows the short-circuit current densities of the gradient doped sample film BPFCO-g under irradiation of 405nm, 520nm, and 650nm light sources, respectively. As can be clearly seen from Figure S6 and Table S3, BPFCO-g film has the highest short-circuit current density under irradiation of 405nm light source. However, its photocurrent density is poorly small under irradiation of light at wavelengths higher than 500 nm.

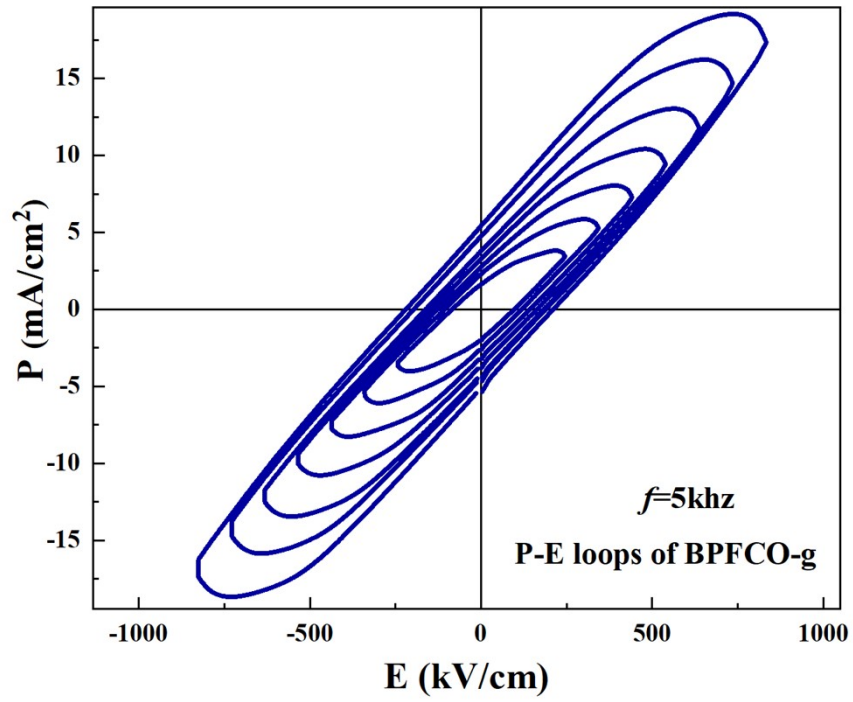


Figure S7. Hysteresis loop of gradient doped sample BPF CO-g

Table S2 Band gap of BPF CO- x ($x=1,2,3$ g) thin films

	BPF CO-1	BPF CO-2	BPF CO-3
Band gap, E_g (eV)	2.41	2.44	2.48