

Supporting Information

# A functional biological molecule restores the $\text{PbI}_2$ residue-induced defects in two-step fabricated perovskites

Yuanmei Huang <sup>1,2</sup>, Guoping Yu <sup>2</sup>, Danish Khan <sup>2</sup>, Shuanglin Wang <sup>3</sup>, Yujie Sui <sup>3</sup>, Xin Yang <sup>1</sup>, Yu Zhuang <sup>1</sup>, Jun Tang <sup>2</sup>, Huaxi Gao <sup>1</sup>, Ming Xin <sup>1</sup>, Abuduwayiti Aierken <sup>1,\*</sup> and Zeguo Tang <sup>2,\*</sup>

<sup>1</sup> School of Energy and Environment, Yunnan Normal University, Juxian Road 768, Chenggong, Kunming 650500, China

<sup>2</sup> College of New Materials and New Energies, Shenzhen Technology University, Lantian Road 3002, Shenzhen 518118, China

<sup>3</sup> College of Materials Science and Engineering, Beijing University of Technology, 100 Pingleyuan, Beijing 100124, China

\* Correspondence: erkin@ynnu.edu.cn (A.A.); tangzeguo@sztu.edu.cn (Z.T.)

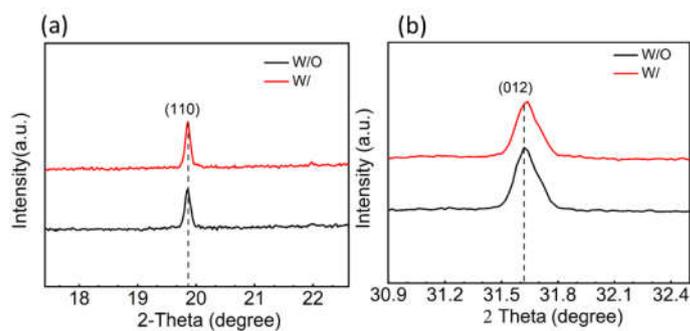


Figure S1: Peak positions for different phases in the control and experimental group, including (PbI<sub>2</sub>) and (001), (110), and (012) phases;

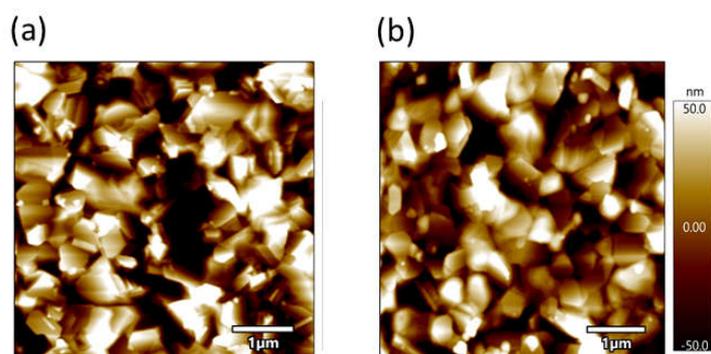


Figure S2: AFM spectra of (a) control and (b) the ART/perovskite layer;

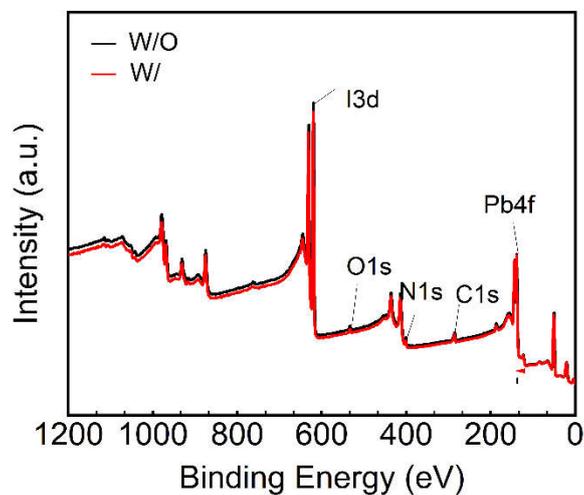


Figure S3: Full XPS spectrum of control and modified perovskite layer;

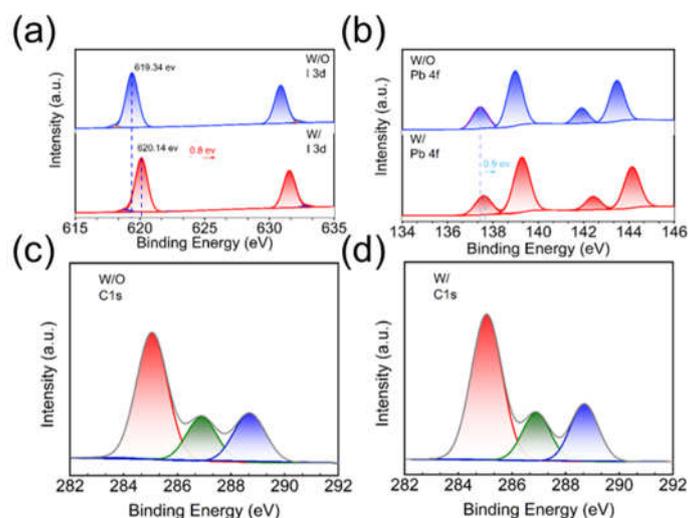


Figure S4: XPS spectra of the control group and experimental group. (a) Peak fitting of I3d peak position change; (b) Peak fitting of Pb4f peak position change; (c) Peak fitting of C1s of the control group (perovskite thin film without artemisinin passivation layer modification); (d) Peak fitting of C1s of the experimental group (perovskite thin film with artemisinin passivation layer modification);

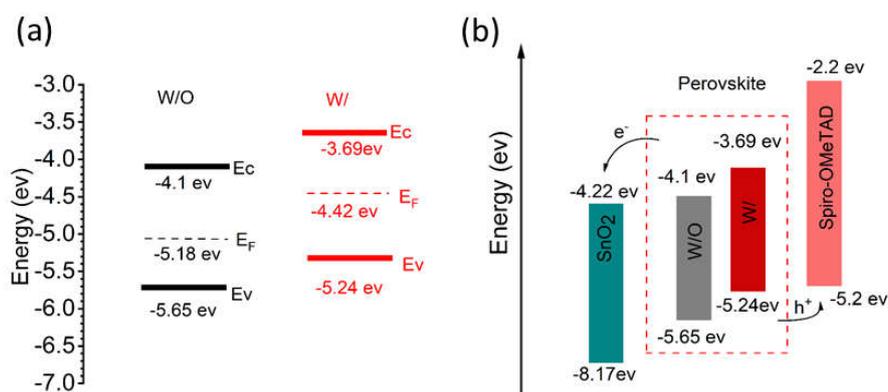


Figure S5: Based on intercepts of the VB region (EB, min) and the SECO region (EB, max) (a) Energy levels and fermi levels (calculated as  $-(21.22 - EB, \max)$  eV; the VBM levels were calculated as  $-(21.22 - EB, \max + EB, \min)$ ) diagrams of perovskite (W/O and W/ ART) (b) The energy levels of all the layers of the device;

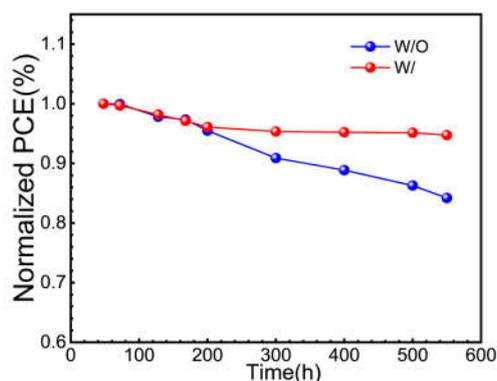


Figure S6: Normalized PCE of the corresponding devices (W/ and W/O ART) kept in N2-glove box (at 25 °C) for 550 h;

Table S1: XPS analysis was used to determine the percentage of surface chemical elements in the control group and the artemisinin passivation layer modified perovskite thin film;

Sample	Pb4f	C1s	O1s	N1s	I3d
W/O	13.96	31.21	6.21	12.43	36.36
W/	13.86	31.88	5.88	10.84	36.19

Table S2: The PL decay curves of the control group and the perovskite thin film modified with artemisinin passivation layer;

Sample	$\tau_1$	$A_1$	$\tau_2$	$A_2$
W/O	394.92	1643.05	2823.17	116.42
W/	509.93	1233.79	565943.52	2443.20

The Table S2 values are measured by using  $(y = A_1 \exp(-\frac{x}{\tau_1}) + A_2 \exp(-\frac{x}{\tau_2}) + y_0)$ .

Table S3: The photoelectric parameters of the control group and the perovskite thin film modified with artemisinin passivation layer;

Sample	Scan direction	$J_{sc}$ (mA/cm <sup>2</sup> )	$V_{oc}$ (V)	FF	PCE (%)
W/O	Forward	24.45	1.08	75.81	20.08
	Reverse	24.86	1.07	75.99	20.21
W/	Forward	24.84	1.11	78.81	21.63
	Reverse	24.69	1.11	79.52	21.72

Table S4: The photoelectric parameters of the control group and the modified with different concentrations of artemisinin in DMSO;

ART ratio in DMSO	Scan direction	$V_{oc}$ (V)	FF (%)	$J_{sc}$ (mA/cm <sup>2</sup> )	PCE (%)
0mg/ml	Forward	1.08	75.81	24.45	20.08
	Reverse	1.07	75.99	24.86	20.21
1mg/ml	Forward	1.11	78.81	24.84	21.63

	Reverse	1.11	79.52	24.69	21.72
	Forward	1.10	77.33	24.26	20.69
1.4mg/ml	Reverse	1.10	76.74	24.26	20.49
	Forward	1.02	77.26	24.57	19.42
2mg/ml	Reverse	1.01	75.42	24.42	18.55

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