

## Supplementary Information

### **Vitamin A as a simple, dual-role agent for the band bending-induced passivation of perovskite solar cells**

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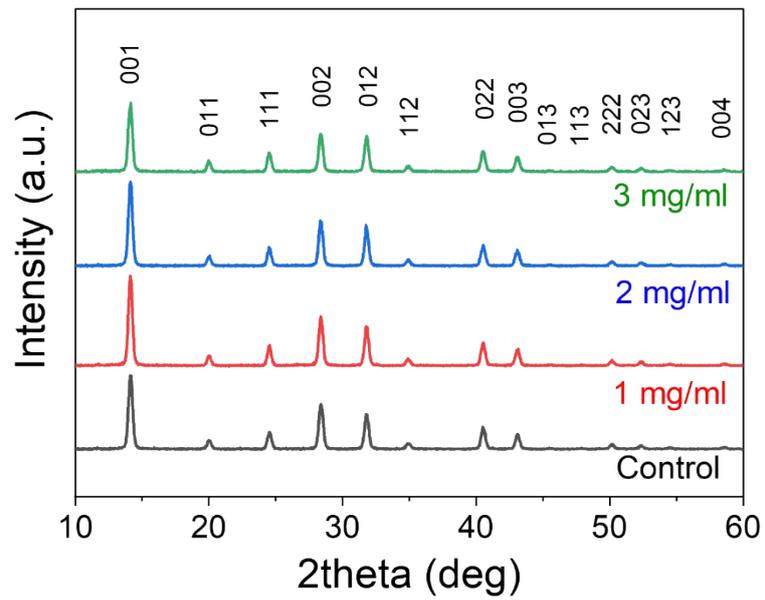


Fig. S1. XRD patterns of perovskite films with 0 (control) 1, 2 and 3 mg/ml of vit A.

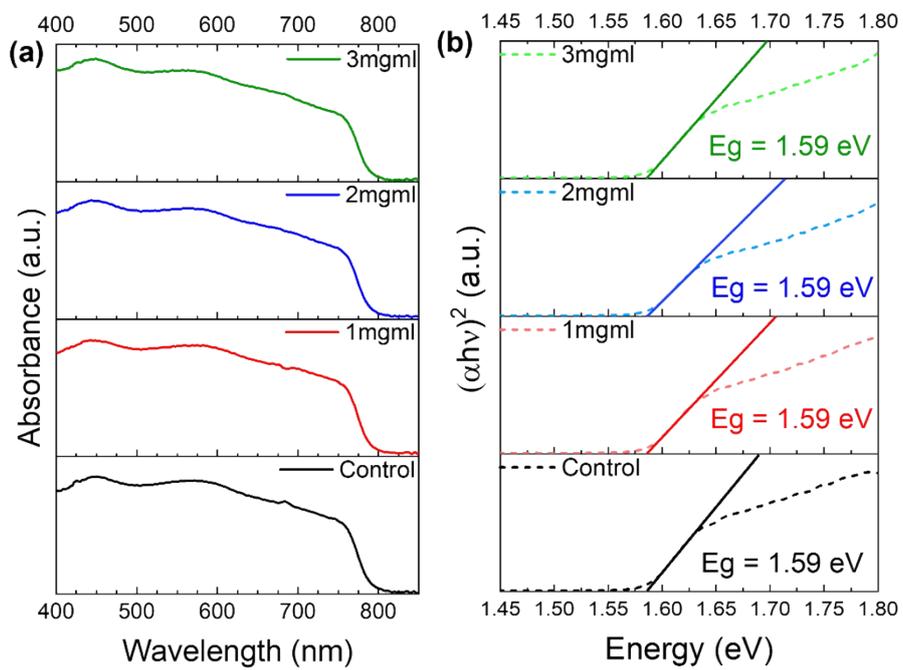


Fig. S2. UV-vis absorption spectrum (a) of perovskite films with 0 (control), 1, 2 and 3 mg/ml of vit A and its corresponding Tauc plots and estimated band gap (b).

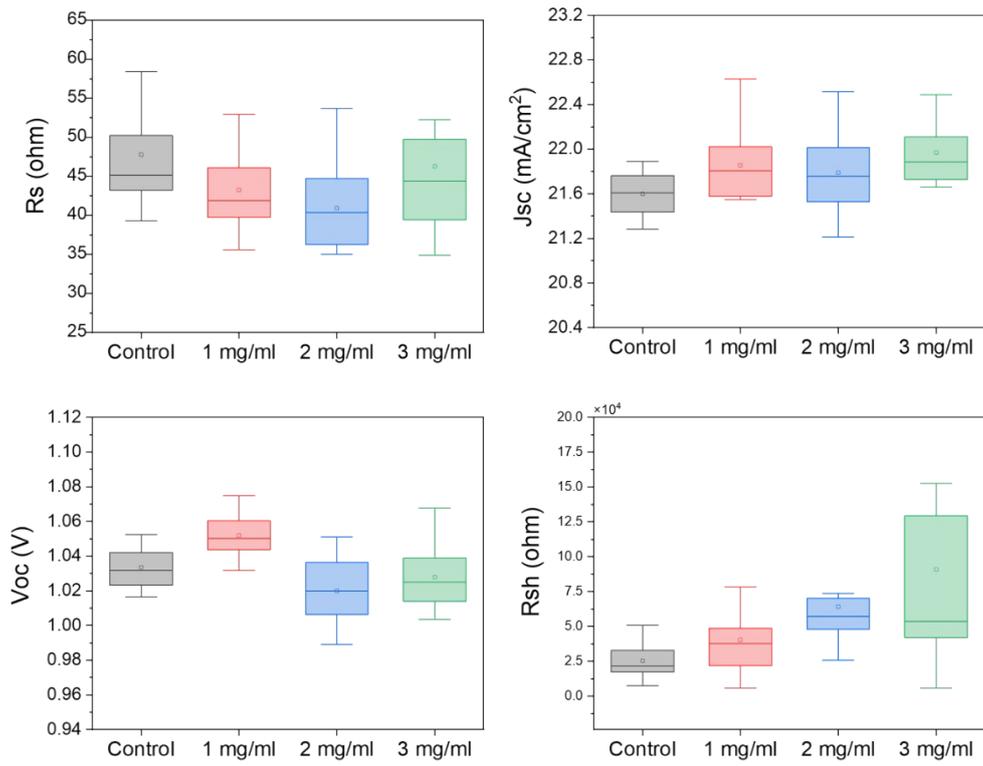


Fig. S3. Photovoltaic property distributions of perovskite solar cells with 0 (control), 1, 2 and 3 mg/ml of vit A.

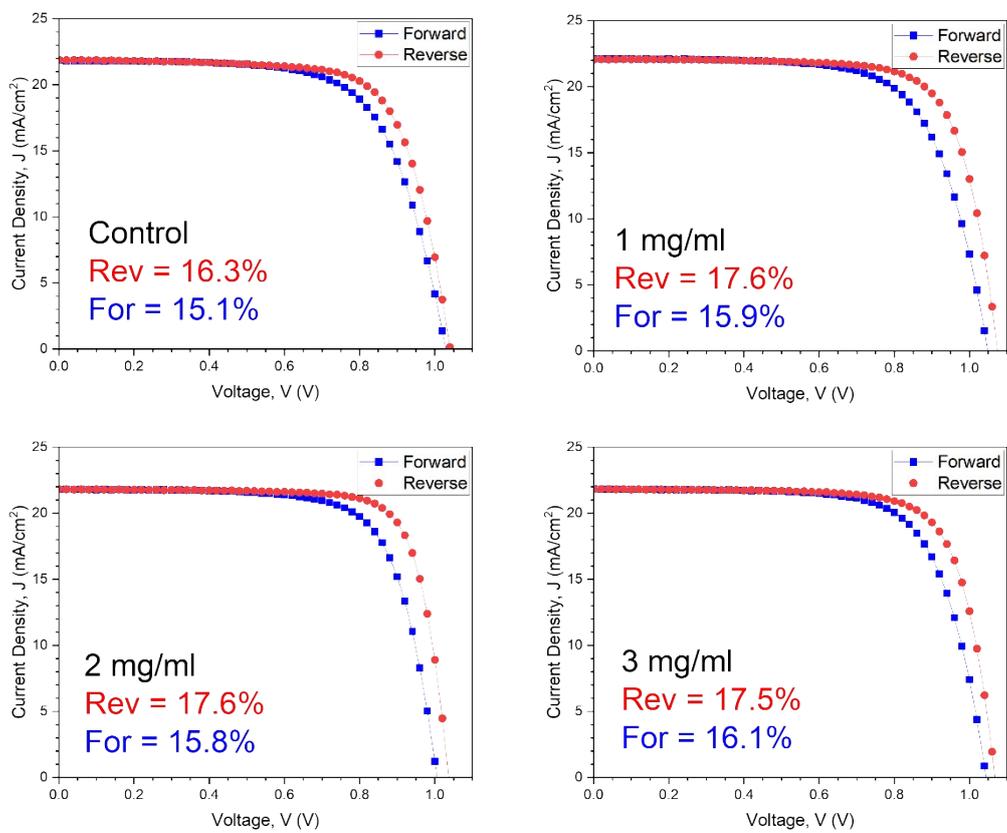


Fig. S4. Forward and reverse J–V scans of the best-performing perovskite solar cell devices with 0 (control), 1, 2, and 3 mg/ml of vit A.

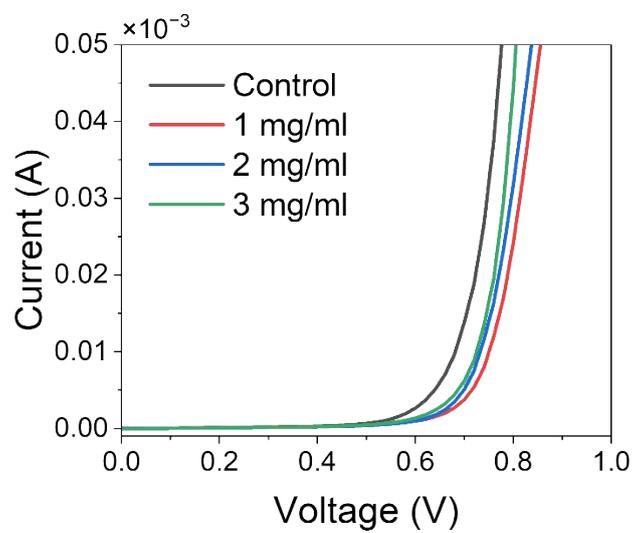


Fig. S5. Dark *J-V* curves of perovskite solar cells with 0 (control), 1, 2 and 3 mg/ml of vit A

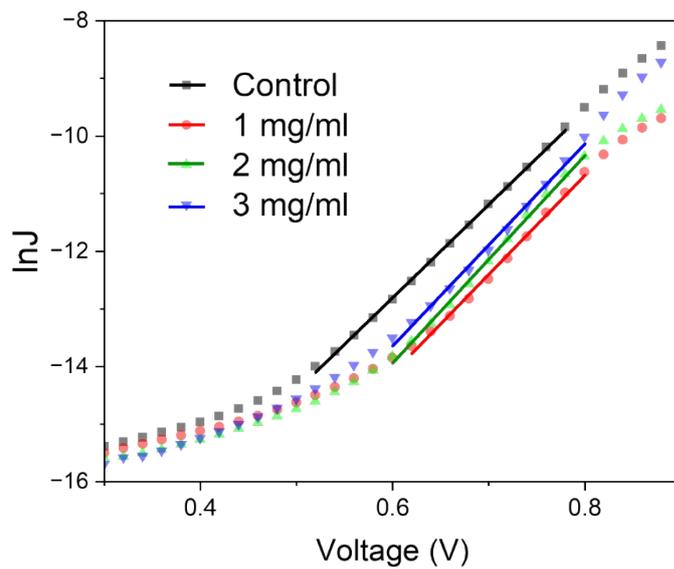


Fig. S6.  $\ln J$  vs.  $V$  for for perovskite solar cells with 0 (control) of 1, 2, and 3 mg/ml of vit A surface treatments. The straight-line segments mark the voltage window used for linear fitting to extract the saturation current density  $J_0$  by the Shockley-diode method. Detailed values of the fitting parameters are listed in Table S1.

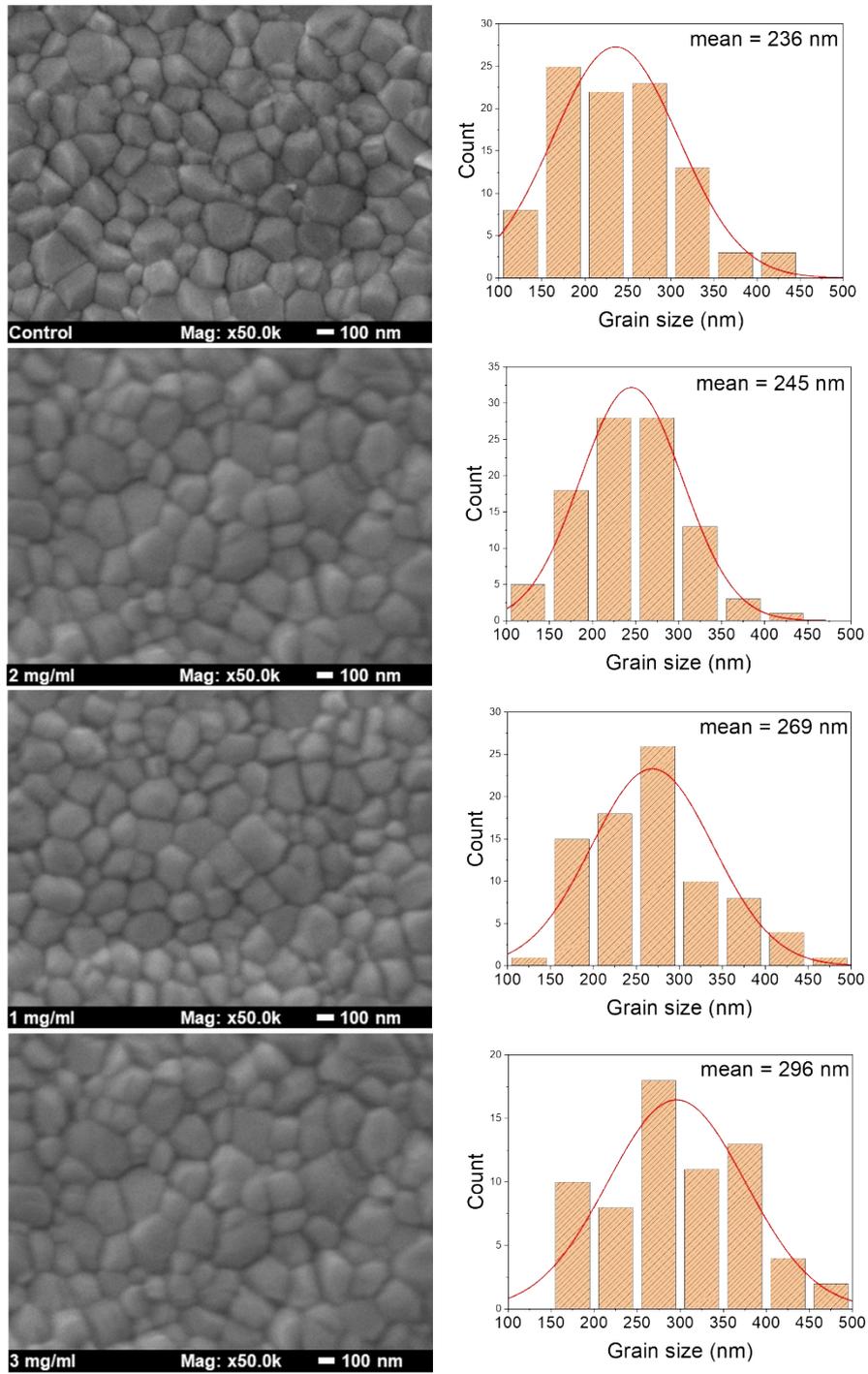


Fig. S7. Scanning electron microscopy (SEM) images of perovskite films with 0 (control), 1, 2 and 3 mg/ml of vit A, and their corresponding grain size distribution. The perovskite film samples were deposited on glass/FTO substrate with SnO<sub>2</sub>.

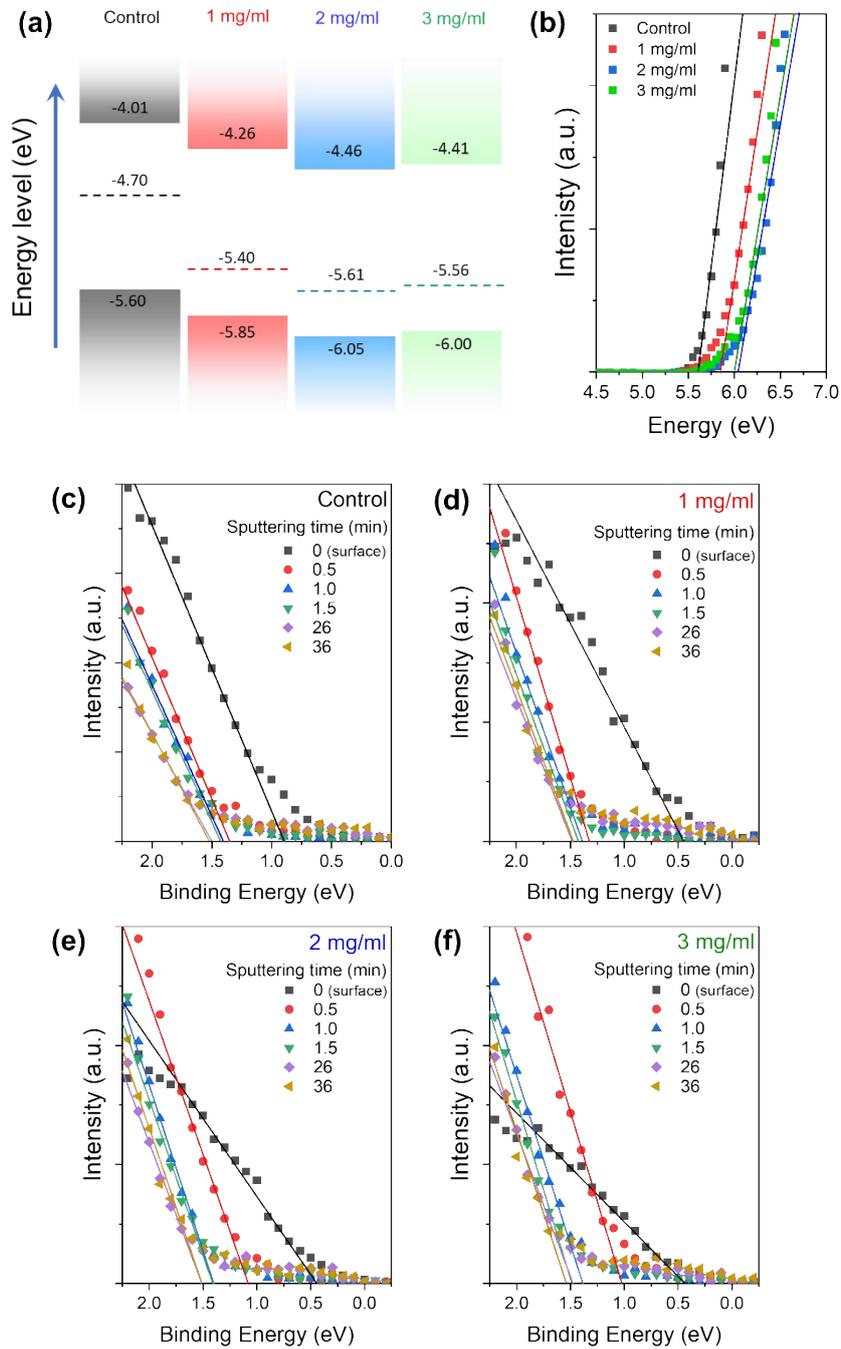


Fig. S8. Band diagram of perovskite films with 0 (control), 1, 2 and 3 mg/ml of vit A (a). Valence band edge values were measured by photoelectron yield spectroscopy (b). Fermi level values of the film surface and the bulk were determined using x-ray photoelectron spectroscopy via surface and depth profile analysis (c-f). The band diagram was completed by using the band gap data in Fig. S2.

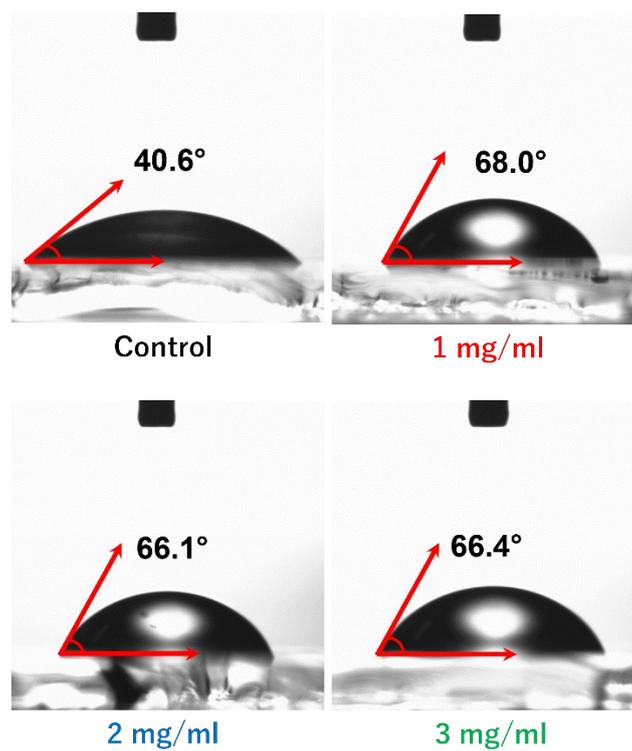


Fig. S9. Representative water-contact-angle images of perovskite films with 0 (control), 1, 2, and 3  $\text{mg ml}^{-1}$  of vit A treatment.

Table S1. Linear-fit results for the semi-log dark J–V curves of perovskite solar cells. Data were fitted with the diode equation expressed in logarithmic form:

$$\ln J = \ln J_0 + \frac{q}{nkT}V$$

where  $J_0 = e^{\text{Intercept}}$  is the saturation current density,  $n$  the ideality factor,  $q$  the elementary charge,  $k$  the Boltzmann constant, and  $T = 300 \text{ K}$ .

<b>Fitted parameter</b>	<b>Control</b>	<b>1 mg mL<sup>-1</sup></b>	<b>2 mg mL<sup>-1</sup></b>	<b>3 mg mL<sup>-1</sup></b>
Intercept, $\ln J_0$	-22.50379	-24.42761	-24.74803	-24.17098
<b><math>J_0</math> (mA cm<sup>-2</sup>)</b>	<b><math>1.7 \times 10^{-10}</math></b>	<b><math>2.5 \times 10^{-11}</math></b>	<b><math>1.8 \times 10^{-11}</math></b>	<b><math>3.2 \times 10^{-11}</math></b>
Slope, $q/nkT$	16.1615	17.1795	18.0090	17.5416
X-Intercept† (V)	1.39243	1.42191	1.37420	1.37792
Reduced $\chi^2$	0.00173	0.00558	0.00348	0.00747
R <sup>2</sup>	0.99913	0.99544	0.99781	0.99506
Pearson r	0.99956	0.99772	0.99891	0.99753

Table S2. Detailed fitting parameters for the time-resolved photoluminescence measurement of perovskite/vit A/HTL films deposited on glass. Excitation wavelength was 425 nm, with the light source directed onto the glass side of the samples. The fitted equation is

$$I = I_0 + A_1 \exp\left(-\frac{(t-t_0)}{\tau_1}\right) + A_2 \exp\left(-\frac{(t-t_0)}{\tau_2}\right)$$

Average time constant ( $\tau_{ave}$ ) was calculated by

$$\tau_{ave} = (A_1\tau_1^2 + A_2\tau_2^2)/(A_1\tau_1 + A_2\tau_2)$$

	<b>Control</b>	<b>1 mg/ml</b>	<b>2 mg/ml</b>	<b>3 mg/ml</b>
$A_1$	7673.72	7841.19	4335.03	4160.23
$\tau_1$ ( $\mu\text{s}$ )	0.02996	0.02379	0.01301	0.01618
$k_{HT}$ ( $\text{s}^{-1}$ )	$3.34 \times 10^7$	$4.20 \times 10^7$	$7.69 \times 10^7$	$6.18 \times 10^7$
$A_2$	2570.39	2846.31	942.97	441.86
$\tau_2$ ( $\mu\text{s}$ )	0.12017	0.07784	0.04942	0.07531
$\tau_{ave}$ ( $\mu\text{s}$ )	0.082	0.053	0.029	0.036
$\tau_{ave}$ (ns)	<b>81.7</b>	<b>53.1</b>	<b>29.5</b>	<b>35.7</b>