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Perovskite ferroelectric thin film as an efficient interface to enhance the photovoltaic characteristics of Si/SnO_x heterojunctions

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Determination of the energy of the Fermi level

The resistivity of the commercial p-/n-type Si substrates is given in Table S1.

Table S1. Resistivity (ρ), dopants concentration (N_D, N_A) and Fermi Level (E_F) for the commercial p-/n-type Si substrates.

	n-Si (Phosporous)	p-Si (Boron)
ρ (Ωcm)	1-6	1-5
N_D (cm^{-3})	8×10^{14}-5×10^{15}	-
N_A (cm^{-3})	-	3×10^{15}-1.5×10^{16}
E_C-E_F (eV)	0.19-0.23	-
E_F-E_V		0.22-0.27 eV

From the resistivity, the donors concentration (N_D for n type) and acceptors concentration (N_A for p type) were estimated from the following equations [1]:

$$\rho = \frac{1}{\sigma} = \frac{1}{q\mu_n N_D}$$

$$\rho = \frac{1}{\sigma} = \frac{1}{q\mu_p N_A}$$

assuming the carriers concentration is equal to doping concentration, q is the elementary charge, σ is the conductivity, μ_n mobility of the electrons and μ_p mobility of the holes.

The mobilities were calculated from the equation [1]:

$$\mu = \mu_{min} + \frac{\mu_{max} - \mu_{min}}{1 + (\frac{N}{N_r})}$$

where the constants are the following ones for the Si dopants [1]:

	Phosphorous	Boron
μ_{min} (cm^2/V-s)	68.5	44.9
μ_{max} (cm^2/V-s)	1414	470.5
N_r	9.20 x 10^{16}	2.23 x 10^{17}
α	0.711	0.719

The Fermi level for p-/n-type Si substrates was then calculated from the equations (2) and (3) in the manuscript and is shown in Table S1.

Determination of the work function

Scanning Kelvin Probe method was used for the determination of the work function (WF) for the p-SnO$_x$ and n-SnO$_x$ films. First we calibrated the system with a gold sample (reference) with well-known work function of 4800 meV. Then, the work function of the tip was obtained taking into account the reference sample and the contact potential difference (CPD) measurement shown in Fig. S1. Thus, the work function of the tip was found to be 4711 meV.

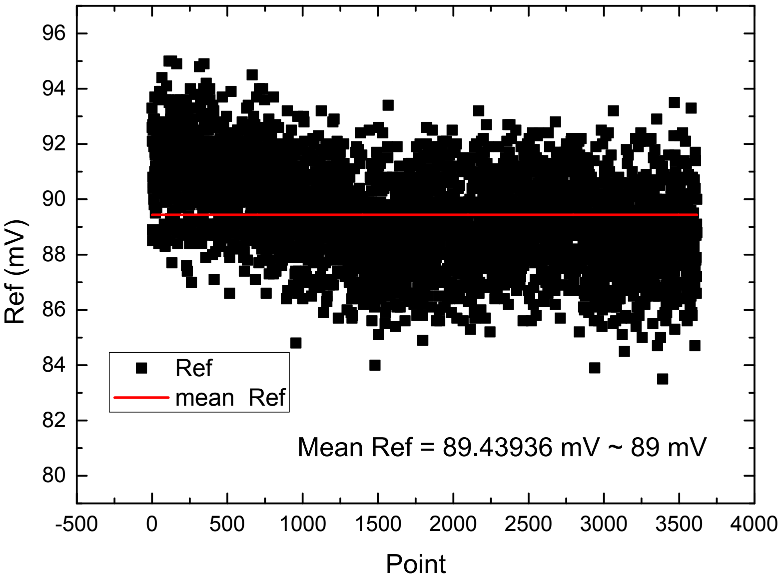

Fig. S1 Contact potential difference measurement of the tip.

After the system calibration, the work function of the p-SnO_x and n-SnO_x films was measured by measuring the CPD signal on each film. Figures S2(a) and (b) show the WF scan profile obtained at the border between the film and the Si substrate for the p-SnO_x and n-SnO_x films, respectively. The WF was found to be ~4.7 eV and ~4.5 eV for the p-SnO_x and n-SnO_x films, respectively.

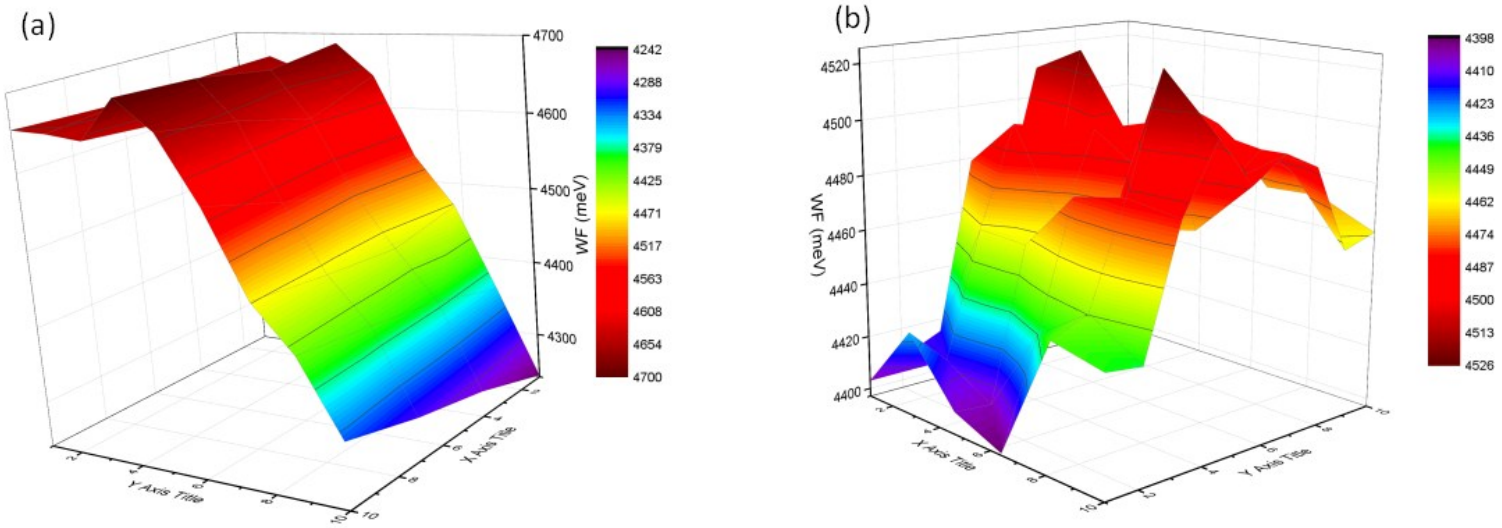

Fig. S2 WF scan profile obtained at the border between the film and the Si substrate for the (a) p-SnO_x and (b) n-SnO_x films, respectively.

Surface photovoltage measurements

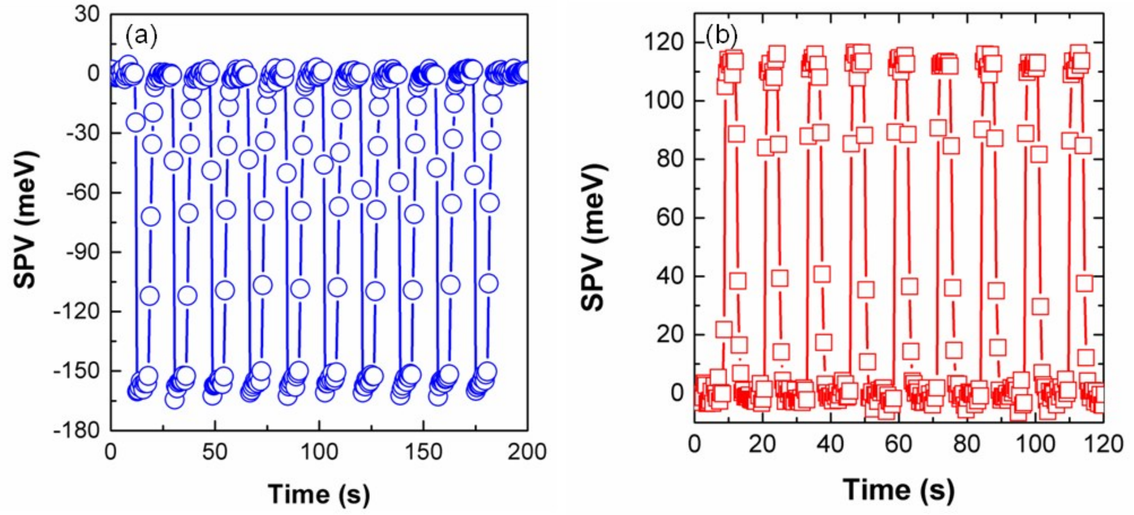

Fig. S3 SPV as a function of time under light excitation pulses for the (a) p-SnO_x and (b) n-SnO_x films, respectively.

References

[1] Bart Van Zeghbroeck, Principles of Semiconductor Devices“ University of Colorado, 2011.