Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supporting Information (SI)

High Efficiency Flexible PEDOT:PSS/Silicon Hybrid Heterojunction Solar Cells Employing Simple Chemical Approach

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(A)

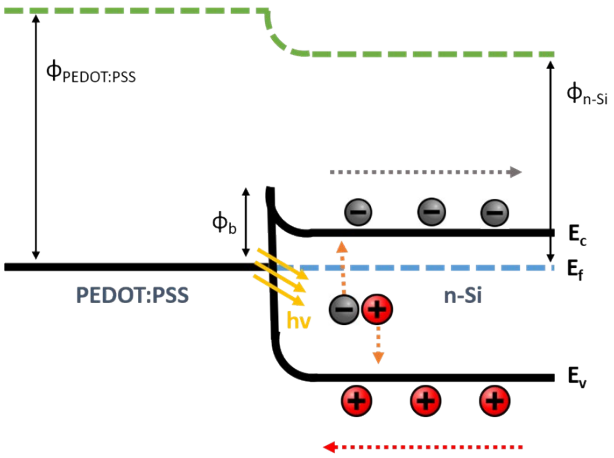


Figure S1. Energy diagram of PEDOT:PSS/n-Si interface.

(B) Silicon wafer etching rate in aq. 20% KOH solution:

The Si wafer of thickness 200±20 µm were thinned down using aq. 20% KOH solution at 75±5 °C temperature. The thickness of wafer at various etching time was noted and plotted in the graph shown below. The required thickness of ~50 µm is obtained by dipping the wafer in alkali solution for 65 min and the etching rate is found to be nearly 2 µm/min.

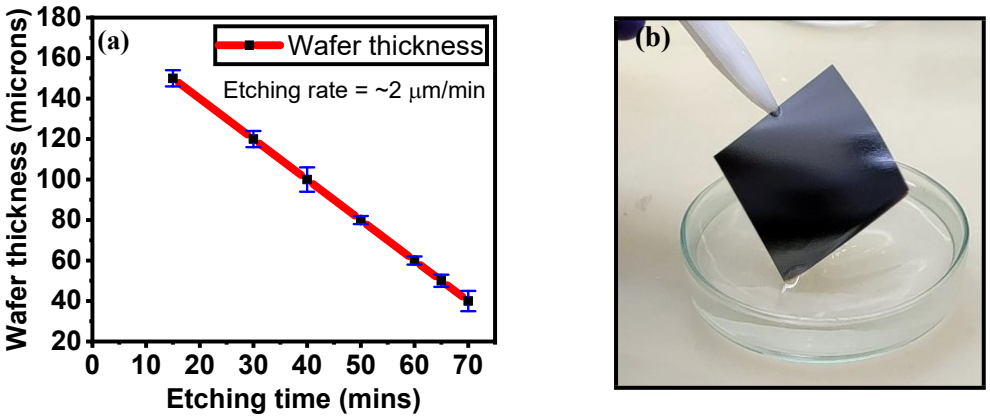


Figure S2. (a) Etching rate estimation from Si wafer thickness vs etching time plot and **(b)** image of thin-flexible Si wafer prepared in laboratory.

(C) Detailed FESEM analysis using ImageJ software for estimating the (i) thickness of wafers (ii) micro-pyramids dimensions and distribution in THSCs with differently textured surfaces:

(i) Untextured (planar) TS_0 surface morphology is shown in Fig. S3 (a) and thickness in Fig. S3 (b) which is ~50 µm. The thickness of different textured TSs were obtained between 50 µm to 40 µm as shown in Fig. S3, so 45±5 µm cells to be fabricated from prepared ~50 µm silicon wafer. Thus, we can say the thickness reduces as texturing time increases and for 60 min i.e., TS_{60} it is 40 µm thin flexible textured Si wafer.

(ii) The height is measured for micro-pyramids on different THSCs surface (Fig. S3 and S4), it is observed that the height of most of micro-pyramid for $THSC_{15}$ ranges from 0.5-2.6 µm, $THSC_{30}$ ranges from 1.4-2.9 µm, $THSC_{45}$ ranges from 2.6-5.0 µm, and $THSC_{60}$ ranges from 3.6-7.4 µm. The size and distribution are shown in Fig. S5.

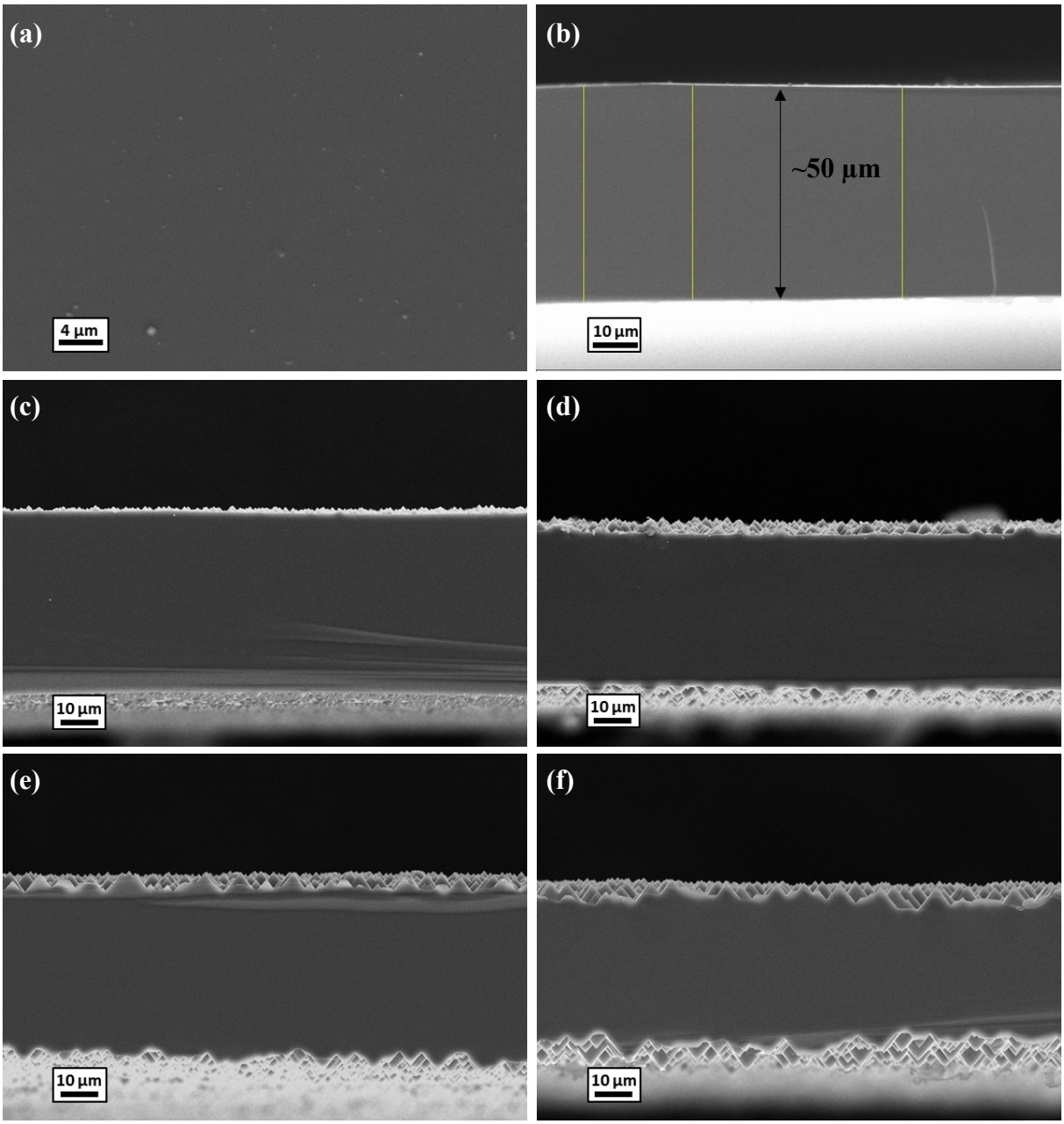


Figure S3. FESEM images showing **(a)** TS_0 [lateral view]; thickness of thin flexible Si wafer [cross sectional view]: **(b)** $TS_{0,}$ **(c)** TS_{15}, **(d)** TS_{30}, **(e)** $TS_{45,}$ **(f)** TS_{60} respectively.

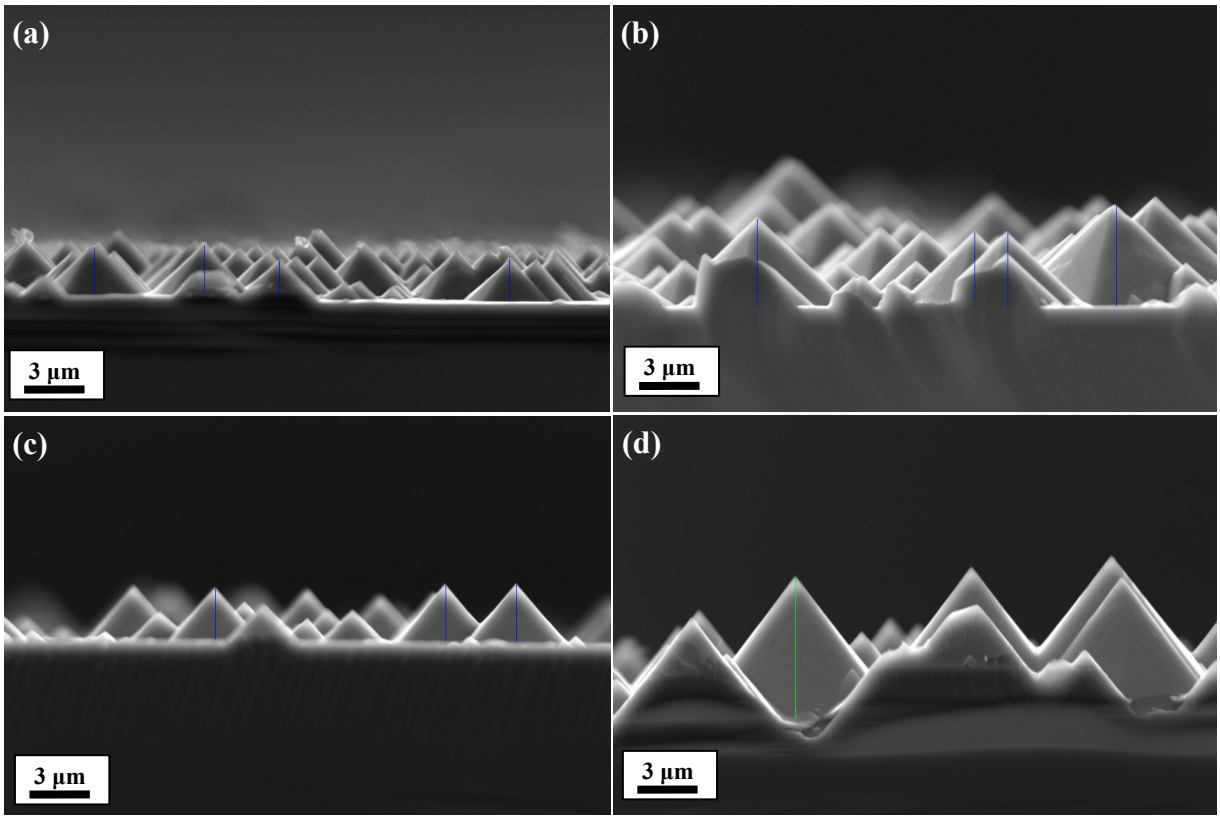
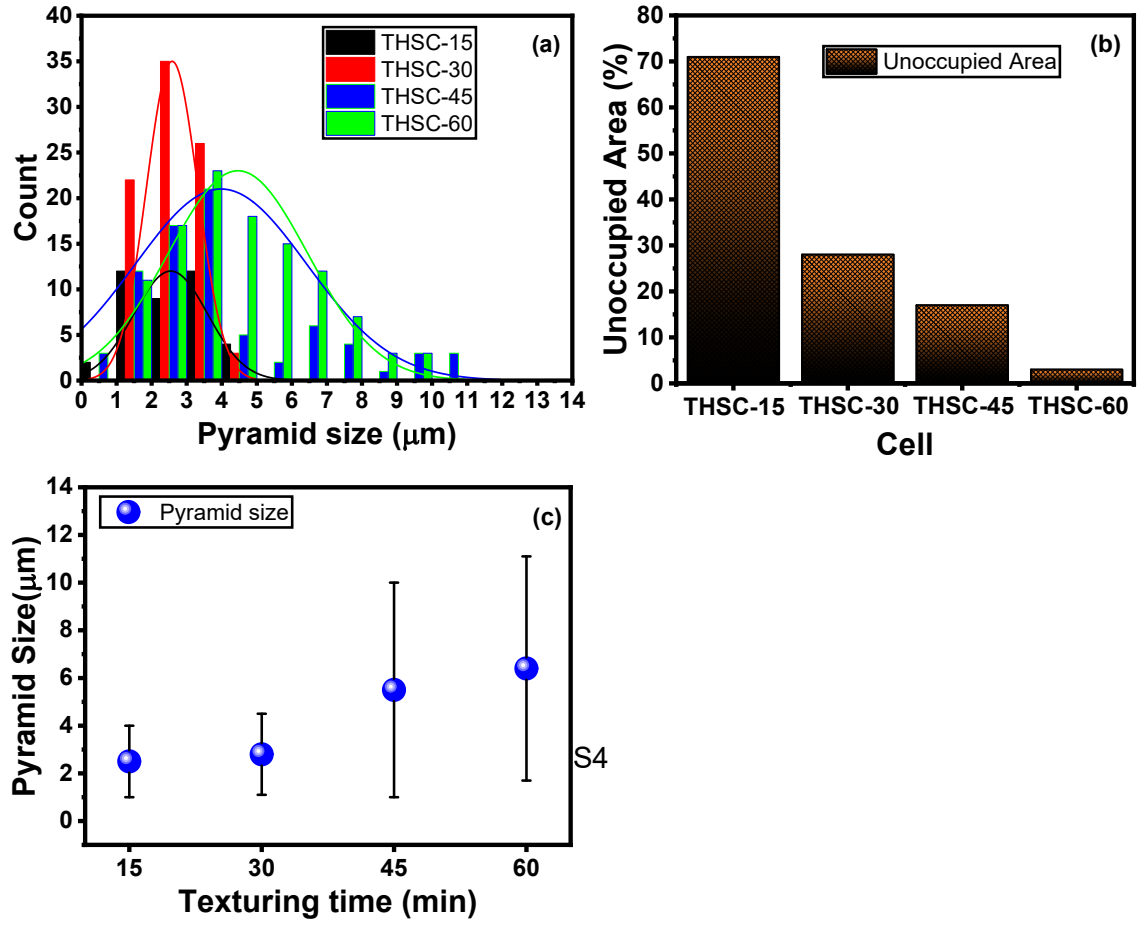


Figure S4. Representative FESEM images (cross sectional view) showing height of pyramid on thin flexible HHSCs (a) $THSC_{15}$, (b) $THSC_{30}$, (c) $THSC_{45}$, (d) $THSC_{60}$ respectively.



S4

Figure S5. Statistically analysed FESEM images for different THSCs for a constant area of 2752 μm^2 using ImageJ, **(a)** Gaussian distribution of the micro-pyramid's base size for different THSCs, **(b)** Percentage area of unoccupancy of micro-pyramids in the surface of different THSCs, **(c)** Variation of average dimension (base) of the micro-pyramids for different THSCs samples.

(D) Optical

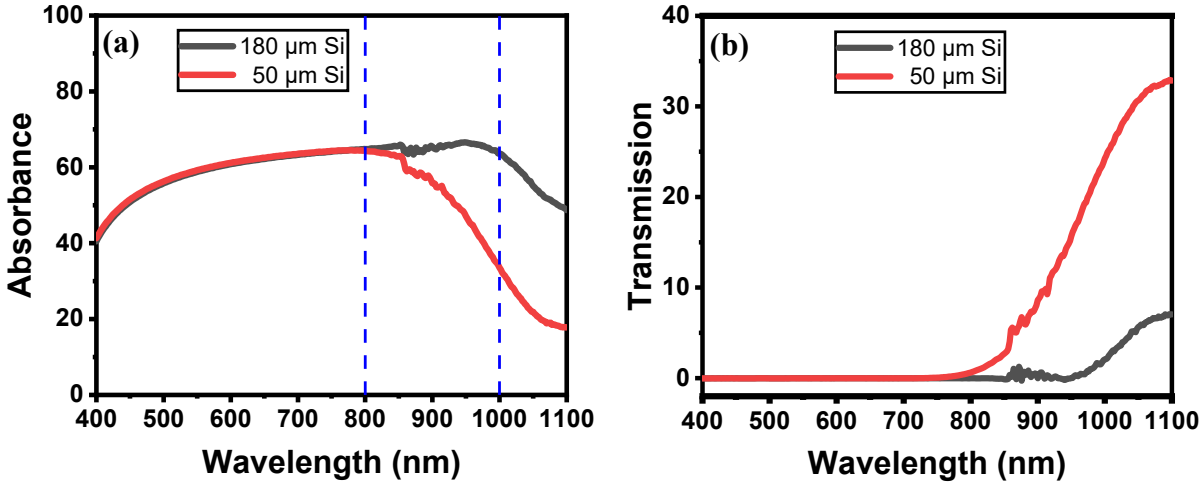


Figure S6. (a) Absorbance and **(b)** Transmission curves for 180 μm thick and 50 μm thin planar Si wafer.

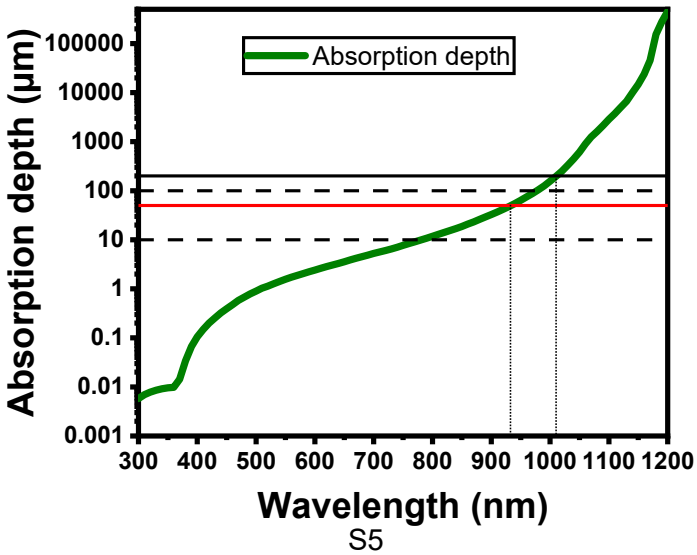


Figure S7. Absorption depth v/s wavelength. **Red** line is for 50 µm thin and **Black** line for 180 µm thick Si wafer.

(E) FDTD Simulation

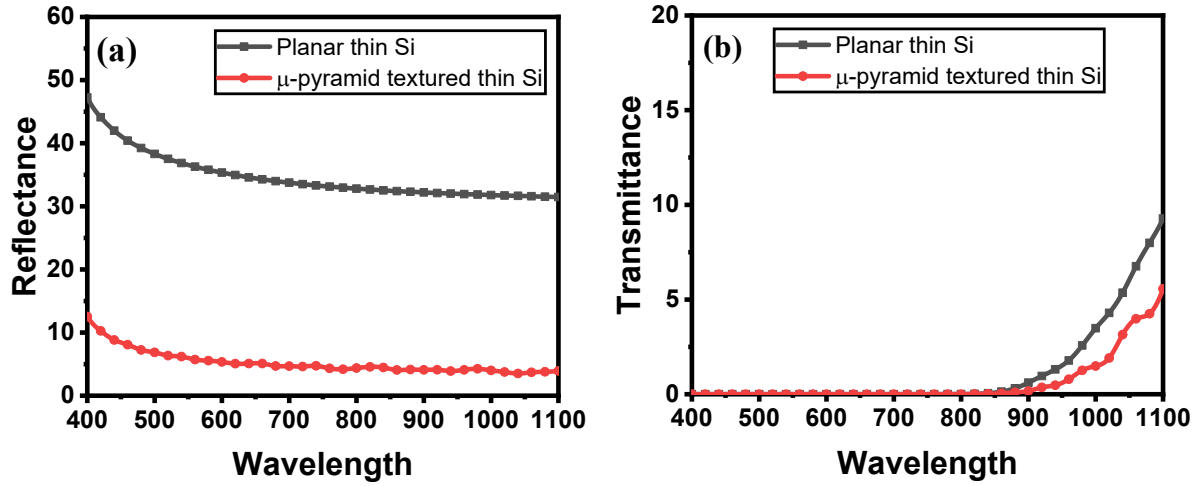


Figure S8. Simulated **(a)** Reflectance and **(b)** Transmittance spectra of planar thin Si and micro-textured thin Si.

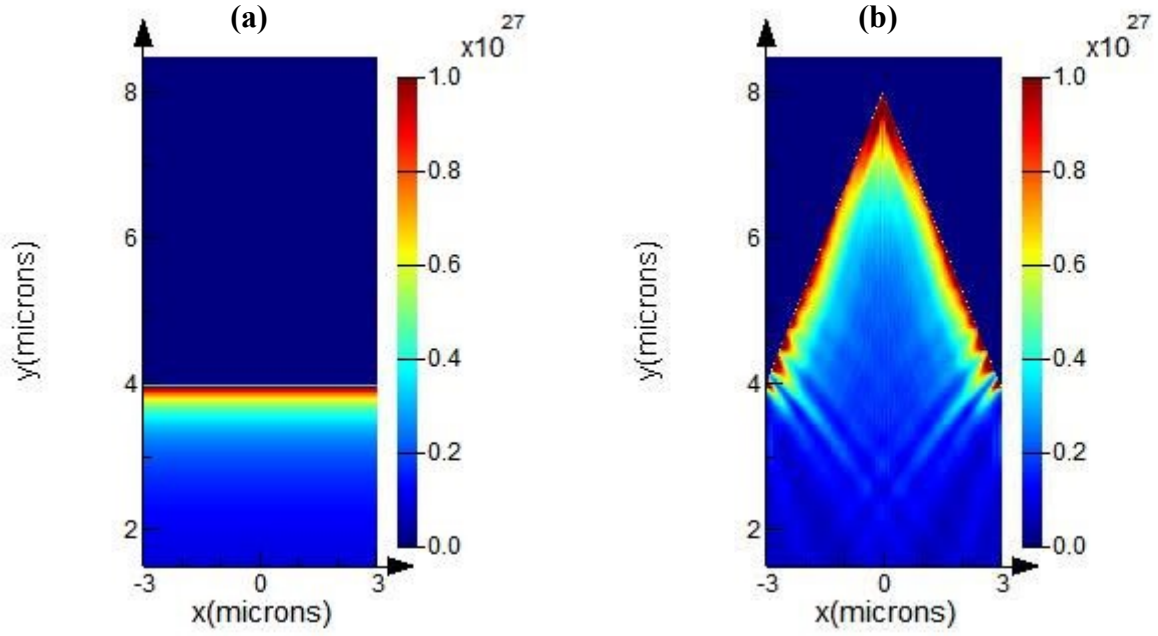


Figure S9. Simulated optical generation rate profile using FDTD for **(a)** planar and **(b)** micro-pyramid textured thin Si.

Table S1: Comparison of MCLT of Si wafers without and with SiO_x layer.

S. No.	Sample details	MCLT (µs)
1.	Bare planar n-Si (without SiO_x)	0.86 ±0.10
2.	SiO_x/planar n-Si/SiO_x	1.03±0.05
3.	PEDOT:PSS/planar n-Si/PEDOT:PSS	7.57±0.77
4.	PEDOT:PSS/SiO_x/planar n-Si/SiO_x/PEDOT:PSS	8.79±0.61

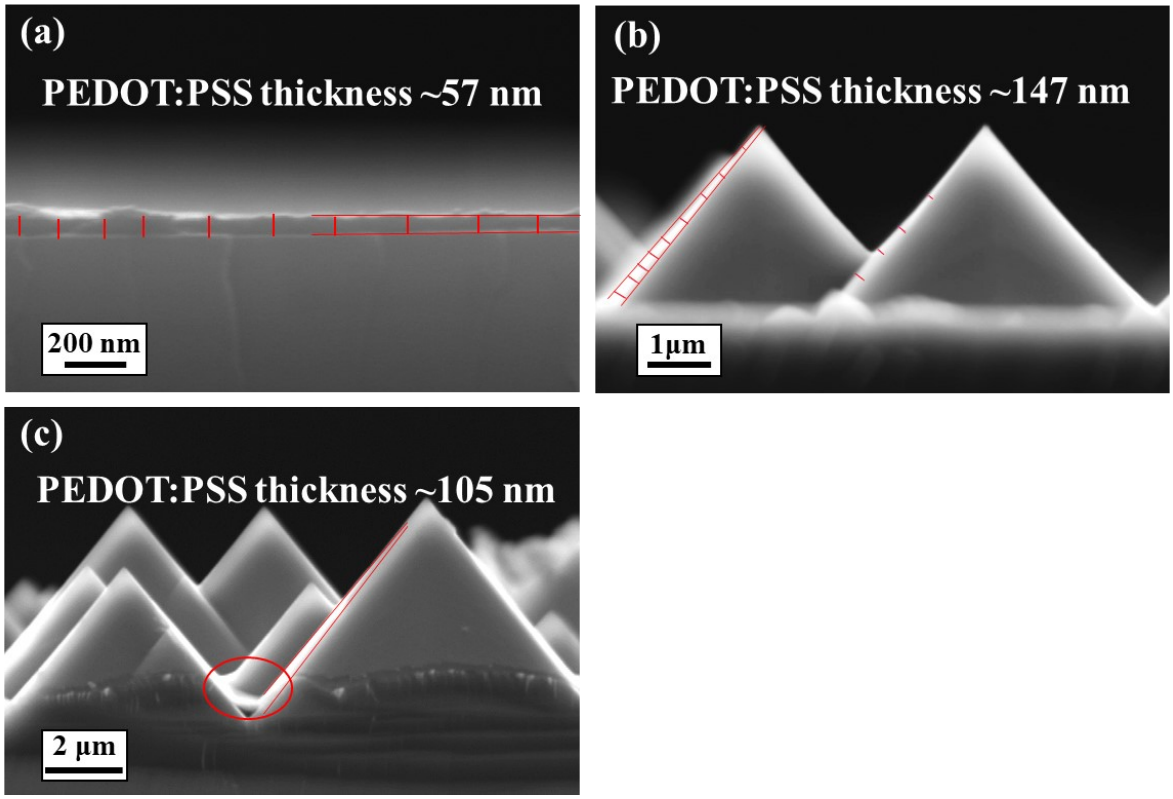


Figure S10. Representative FESEM image showing PEDOT:PSS thickness on **(a)** TS_0, **(b)** TS_{30}, and **(c)** TS_{60} samples.

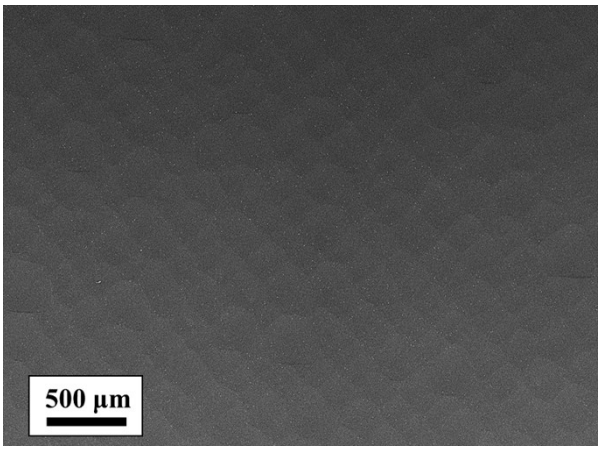


Figure S11. Representative high magnification FESEM image for Si wafer after aq. KOH thinning.

Table S2. PV performance parameters of THSCs fabricated on three different batches with statistical analysis. The 'Batch 3' parameters are chosen in the main manuscript for comparative analysis and discussion.

Solar Cell and performance parameters		**Batch 1**	**Batch 2**	**Batch 3 (champion PCE cell batch)**		**Statistics of 3 batches**
$THSC_0$	V_{oc} (V)	0.498±0.005	0.478±0.007	0.498±0.010	**0.507**	0.491±0.012
	J_{sc} (mA/cm^2)	20.16±0.29	19.02±0.06	20.61±0.47	**20.40**	19.93±0.51
	FF (%)	36.30±4.65	49.40±0.92	37.31±7.40	**43.64**	41.00±6.55
	PCE (%)	4.03±0.33	4.49±0.23	3.84±0.85	**4.51**	4.12±0.32
$THSC_{15}$	V_{oc} (V)	0.481±0.006	0.473±0.004	0.493±0.005	**0.493**	0.482±0.008
	J_{sc} (mA/cm^2)	21.60±0.57	22.92±0.61	22.91±1.69	**21.86**	22.47±1.37
	FF (%)	46.05±1.68	46.42±3.98	46.26±2.48	**46.03**	46.24±2.23
	PCE (%)	4.77±0.07	4.80±0.13	5.23±0.55	**4.96**	4.93±0.29
$THSC_{30}$	V_{oc} (V)	0.484±0.004	0.487±0.017	0.498±0.004	**0.494**	0.490±0.007
	J_{sc} (mA/cm^2)	23.81±0.40	22.05±0.84	22.85±1.04	**24.06**	22.90±0.97
	FF (%)	45.97±3.13	60.80±3.80	51.70±2.22	**52.13**	52.82±6.83
	PCE (%)	5.29±0.23	6.61±0.69	5.88±0.36	**6.19**	5.93±0.71
$THSC_{45}$	V_{oc} (V)	0.516±0.010	0.511±0.004	0.507±0.006	**0.512**	0.511±0.006
	J_{sc} (mA/cm^2)	25.94±0.43	25.13±0.21	25.10±1.40	**26.02**	25.39±0.40
	FF (%)	62.03±3.12	64.04±1.49	58.23±4.37	**62.51**	61.43±2.39
	PCE (%)	8.30±0.43	8.25±0.20	7.43±0.94	**8.33**	7.99±0.34
$THSC_{60}$	V_{oc} (V)	0.528±0.002	0.526±0.002	0.524±0.003	**0.522**	0.526±0.003
	J_{sc} (mA/cm^2)	25.07±1.91	25.34±0.71	28.35±0.65	**28.75**	26.25±1.33
	FF (%)	67.89±1.14	69.57±3.56	66.53±4.22	**69.45**	67.99±1.47
	PCE (%)	8.99±0.33	9.30±0.63	9.89±0.87	**10.42**	9.39±0.76

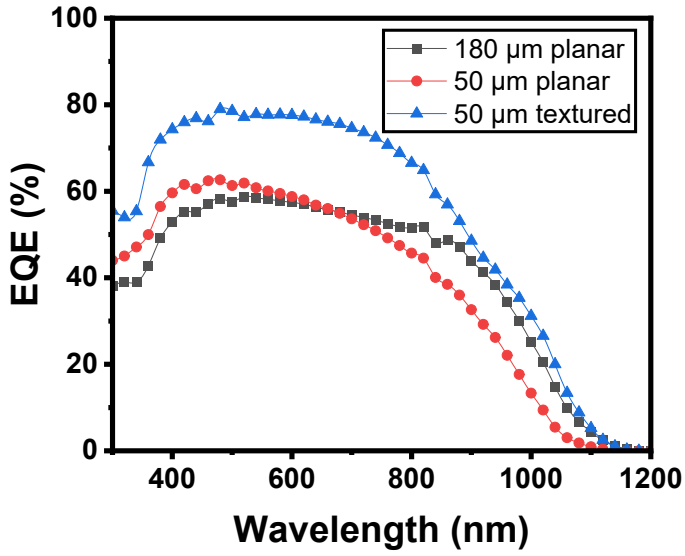
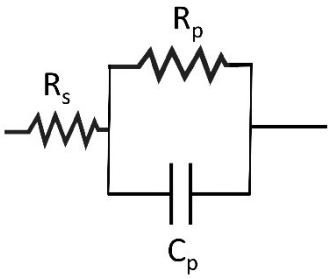


Figure S12. EQE spectra for HHSC prepared on 180 µm, 50 µm ($THSC_0$) untextured Si wafer; and 50 µm textured ($THSC_{60}$).

(E) EIS (Electrochemical Impedance Spectroscopy)

Complex impedance



Resultant impedance of R_p and C_p is

$$\frac{1}{Z} = \frac{1}{R_p} + \frac{1}{\chi_p}$$

$$\Rightarrow \frac{1}{Z} = \frac{1}{R_p} + j\omega C_p$$

$$\Rightarrow Z = \frac{R_p}{1 + j\omega C_p R_p}$$

Realising it we get,

$$\Rightarrow Z = \frac{R_p}{1 + (\omega C_p R_p)^2} - j\frac{\omega C_p R_p^2}{1 + (\omega C_p R_p)^2}$$

Here we getting the real and imaginary part of resultant impedance. The imaginary impedance is in negative axis. Now. If series resistance is considered then we obtain

$$Z^{'} = R_s + \frac{R_p}{1 + (\omega C_p R_p)^2} \quad \text{…. (i)}$$

$$Z^{''} = \frac{\omega C_p R_p^2}{1 + (\omega C_p R_p)^2} \quad \text{…. (ii)}$$

from equation (i), we get

$$Z^{'} - R_s = \frac{R_p}{1 + \left(\frac{R_p}{\chi_p}\right)^2} = \frac{\chi_p^2 R_p}{\chi_p^2 + R_p^2} \quad \text{…. (iii)}$$

from equation (ii), we get

$$Z^{''} = \frac{R_p^2 \frac{1}{\chi_p}}{1 + \left(\frac{R_p}{\chi_p}\right)^2} = \frac{R_p^2 \chi_p}{\chi_p^2 + R_p^2} \quad \text{…. (iv)}$$

Squaring and adding equation (iii) and (iv),

$$\left(Z^{'} - R_S\right)^2 + \left(Z^{''}\right)^2 = \frac{\left(\chi_p^2 R_p\right)^2 + \left(R_p^2 \chi_p\right)^2}{\left(\chi_p^2 + R_p^2\right)^2}$$

$$= \frac{\chi_p^2 R_p^2}{\chi_p^2 + R_p^2}$$

$$= R_p \frac{\chi_p^2 R_p}{\chi_p^2 + R_p^2}$$

$$= R_p (Z^{'} - R_s)$$

Thus, we obtain

$$R_p = \frac{\left(Z^{'} - R_s\right)^2 + (Z^{''})^2}{\left(Z^{'} - R_s\right)}$$

Similarly, we can find

$$\chi_p = \frac{\left(Z^{'} - R_s\right)^2 + (Z^{''})^2}{Z^{''}}$$

$$C_p = \frac{1}{\omega \chi_p} = \frac{1}{2\pi f \chi_p}$$

So,

C_p is fitted at such frequency where Z'' has maximum value.