Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Role of MoS_2 as interfacial layer in graphene/silicon solar cells

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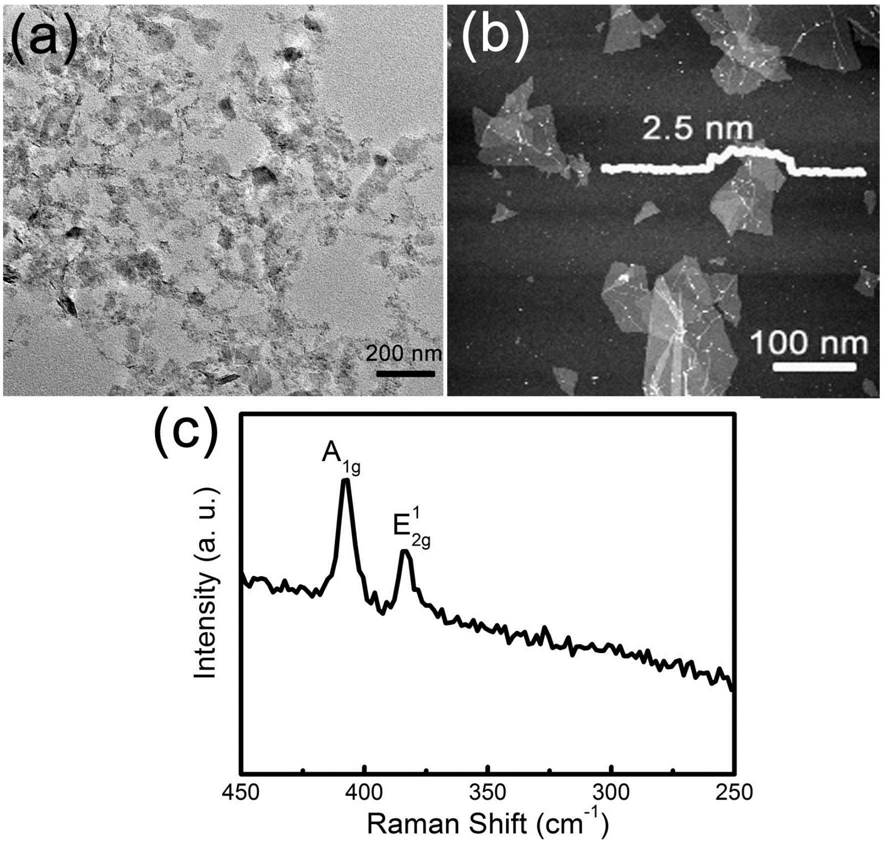

Fig. S1. Characterizations of MoS_2 nanoflakes (a) TEM, (b) AFM, (c) Raman Spectrum

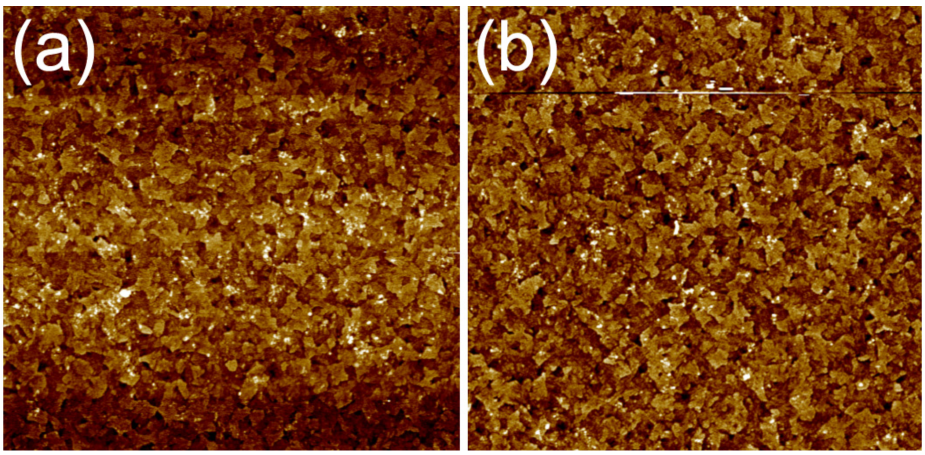

Fig. S2. AFM images of MoS_2 films deposited on Si substrates. (a) MoS_2 (80) film, (b) MoS_2 (200) film. Clearly the Si substrate is uniformly covered by MoS_2 and there are little changes in the morphologies of MoS_2 (80) and MoS_2 (200) films.

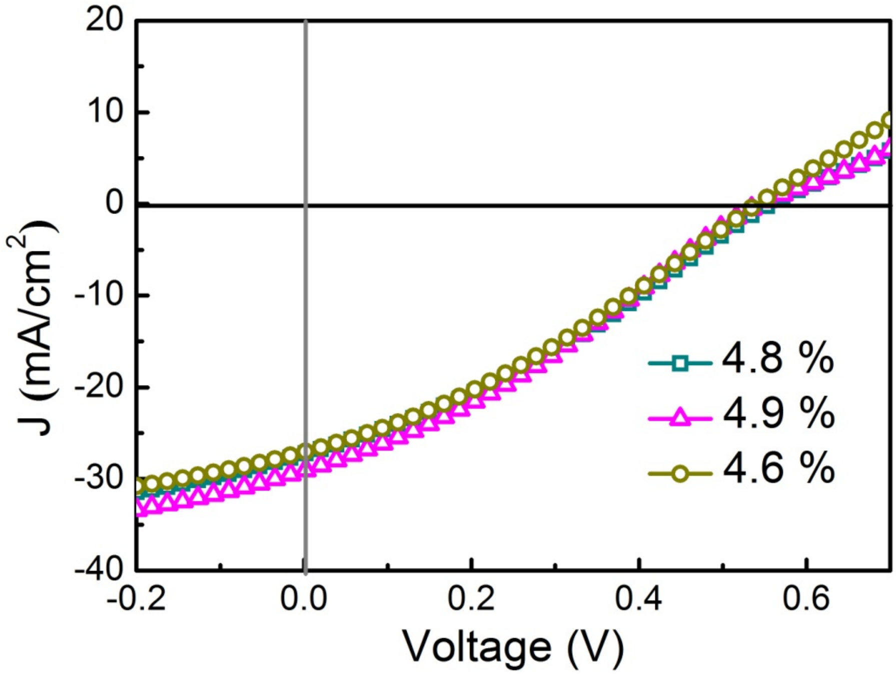

Fig. S3. I-V curves of G/MoS_2(80, Ar)/n-Si devices. The PCE of G/MoS_2(80, Ar)/n-Si is very close to that of G/MoS_2(80)/n-Si device, indicating that the improvements in PCE has nothing to do with SiOx layer, but solely due to the MoS_2 interfacial layer.

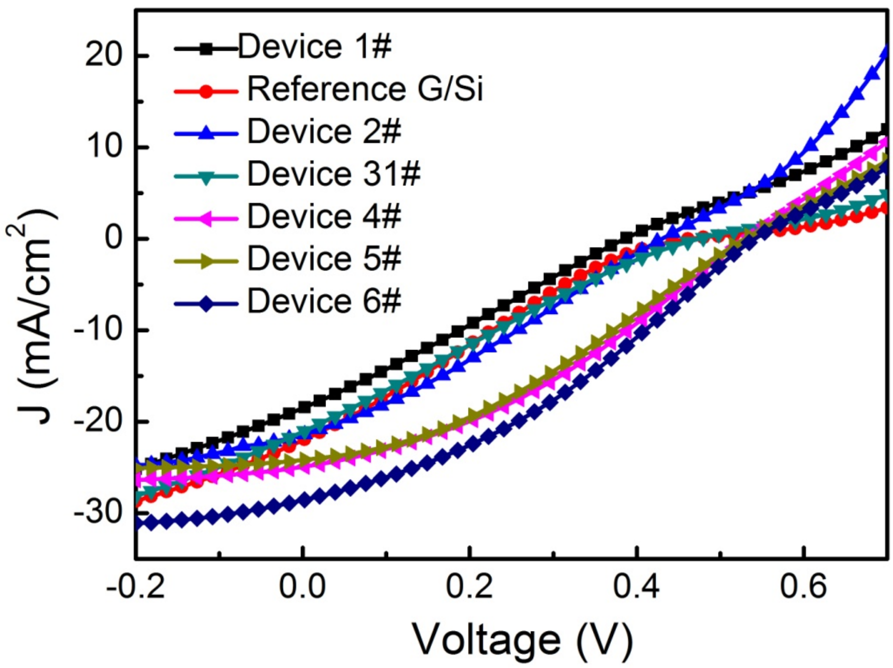

Fig. S4. I-V curves of G/MoS_2/n-Si devices without thermal treatments. The fluctuations in PCE are ascribed to the instability of un-annealed MoS_2 films when coming into contact with water.

Discussions on Fig. S4

As can be seen from Fig. S4 and Table S2, there are fluctuations in PCE. We fabricated six parallel devices and it is found that three of them show enhancements in PCE (~5 %) while the other three shows no improvements. It is plausible that the interactions between silicon and un-annealed MoS_2 are not stable enough to give reliable PCE (Note that the graphene is transferred onto silicon using wet-transfer method, so un-annealed MoS_2 films tends to be unstable when coming into contact with water, leading to the fluctuations in PCE). Though the PCE is not stable, it can also be used to exclude the effects of SiO_x. That is, when the MoS_2 films are not damaged when exposing to water, it can improve the PCE effectively.

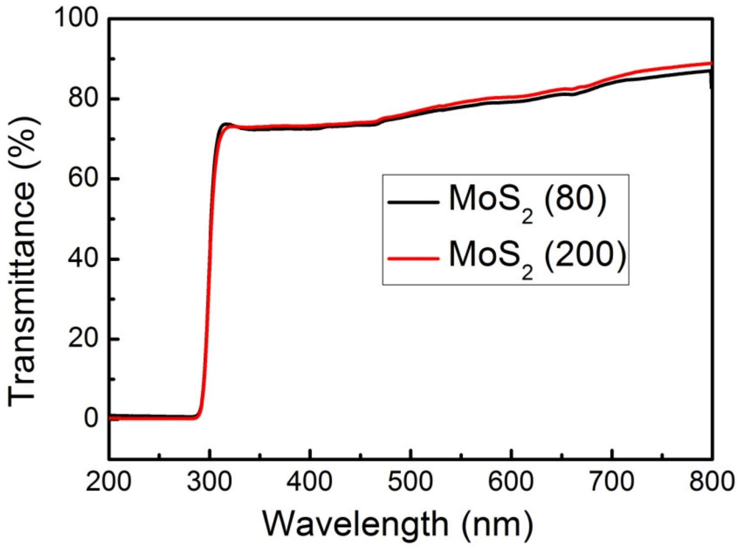

Fig.S5. The transmittance spectra of MoS_2(80) and MoS_2(200) films. The measurments are carried out as follows: First MoS_2 nanoflake solution is drop-casted onto glass and baked at 80 ^oC for 15 min. Then the transmittance spectra is measured (i.e., the transmittance spectra of MoS_2 (80) film). The glass is then annealed at 200 ^oC under the protection of Ar for 15 min and the transimttance spectra of MoS_2(200) is obtained. Clearly there is little change for the same MoS_2 film with different annealing temperature.

Table S1. Device parameters of solar cells in Fig. S3.

	J_{sc} (mA/cm^2)	V_{oc} (V)	FF	PCE (%)
Green line	27.2	0.55	0.32	4.8
Pink line	29	0.54	0.32	4.9
Tawny line	27	0.54	0.32	4.6

Table S2. Device parameters of solar cells in Fig.S4.

	J_{sc} (mA/cm^2)	V_{oc} (V)	FF	PCE (%)
1 #	18.4	0.37	0.28	1.88
2 #	21.9	0.46	0.23	2.31
3 #	21.3	0.42	0.29	2.65
4 #	24.9	0.52	0.36	4.62
5 #	26.8	0.52	0.35	4.84
6 #	28.6	0.54	0.35	5.30

Table S3. Calculated device parameters of solar cells in Fig. 1

Ann.Temp. (^{o}C)	SBH (eV)	n	Rs1(Ω)	Rs2(Ω)
Ref.	0.64	2.24	586.3	597.8
80	0.72	2.25	155.7	160.0
200	0.65	2.57	593.0	592.2

Footnotes: R_{s1} and R_{s2} are calculated respectively from the dV/d(lnJ) vs J plot and H(J) vs J plot to see the consistency of the method.

Table S4. MoS_2 film thickness measured by ellispometer.

	1	2	3	**Average (nm)**
Green Curve	1.87	1.72	1.80	**1.80**
Blue Curve	2.38	2.45	2.40	**2.41**
Red Curve	3.60	3.55	3.58	**3.58**
Black Curve	4.62	4.60	4.59	**4.60**

Table S5. Photovoltaic parameters of devices in Fig. 8.

δ (nm)	V_{oc} (V)	J_{sc} (mA/cm^2)	FF	PCE (%)
4.60	0.5	19.6	0.27	2.63
3.58	0.52	23.1	0.30	3.65
2.41	0.5	27.2	0.32	4.45
1.80	0.52	27.0	0.32	4.50