Interface engineering and efficiency improvement of monolayer graphene-silicon solar cells by inserting an ultra-thin LiF interlayer

Dikai Xu, Xuegong Yu*, Lijian Zuo, Deren Yang

Supporting Information

1. Extraction the values of series resistances of solar cells

Relation between current density and voltage (*J-V*) under dark condition can be expressed by equation (S1.1) when series resistance (R_s) is taken into account, [1-3]

$$J = J_s(\exp(\frac{q(V - JR_s)}{nkT}) - 1) \quad \text{(S1.1)}$$

where J_s is the reversed saturation current density, T the absolute temperature (298 K) and V-JR_s the voltage applied across the Schottky solar cells. For $V - JR_s > 3kT/q$, the *J-V* relation becomes as follows,

$$J = J_s \exp\left[\frac{q(V - JR_s)}{nkT}\right] \quad \text{(S1.2)}$$

Equation (S1.2) can be differentiated and rearranged into formula as follows,

$$\frac{dV}{d(\ln J)} = R_s A_{eff} J + \frac{nkT}{q} \quad \text{(S1.3)}$$

where A_{eff} is effective area of Schottky solar cells. The value of R_s is obtained from slope of dV/d(ln$J$) versus J curves.

2. Calculation of the values of contact resistances

The values of contact resistance, ρ_C, for the Al/Si direct contact and the Al/LiF/Si contact, are extracted by the transmission line model method.[4] Detailed extraction process is described as follows. Current-voltage (*I-V*) curves between two contacts with length *d* and width *W* were measured by a probing station. As shown in the inset of Figure 5, the distance between Al electrodes were 100, 200, 300, *etc.* then finally 600 μm. The total resistances, R_T, between every two electrodes are derived from the *I-V* curves, correspondingly. The contact resistance, R_C, can be obtained by fitting equation (S2.1) as follows,

$$R_T = 2R_C + R_{sh} l/W \tag{S2.1}$$

where the R_{sh} is the sheet resistance of Si and *l* the distances between two electrodes. The value of L_T is obtained by equation (S2.2) and (S2.3) as follows,

$$R_E = \frac{1}{2}(R_1 + R_2 - R_3) \tag{S2.2}$$

$$R_C / R_E = \cosh(d/L_T) \tag{S2.3}$$

where R_E is the contact end resistance, L_T the transfer length and *d* the length of electrodes. Schematic diagram of R_1, R_2 and R_3 is shown in Figure S1. Eventually, ρ_C is extracted from equation (S2.4),

$$\rho_C = R_E L_T W \sinh(d/L_T) \tag{S2.4}$$

The calculated contact resistances for the Al/Si and Al/LiF/Si contact were 1.9×10^{-1} Ω cm^2 and 6.3×10^{-2} Ω cm^2, respectively.

Table S1. Summary of photovoltaic parameters of devices with 0.5 nm and 1.2 nm LiF interlayer fabricated in the same batch.

Nominal thickness Of LiF interlayer	V_{OC} (mV)	J_{SC} (mA/cm^2)	*FF* (%)	PCE (%)
1.2 nm	403.86	24.93	45.00	4.53
	386.28	26.74	44.58	4.60
	405.20	26.18	46.15	4.89
0.5 nm	400.42	26.29	53.06	5.58
	405.34	24.83	54.50	5.48
	430.97	27.17	49.66	5.81

Table S2. Summary of photovoltaic parameters of devices during one week storing.

Gr-Si Solar cells	Storing time (day)	V_{OC} (mV)	J_{SC} (mA/cm^2)	*FF* (%)	PCE (%)
Pristine-1	0	327.75	24.30	45.23	3.60
	1	400.21	25.50	53.45	5.45
	2	389.11	25.08	53.18	5.19
	3	405.34	24.83	54.50	5.48
	7	438.45	24.40	50.18	5.37
Pristine-2	0	347.26	27.70	47.57	4.58
	1	408.61	27.03	54.95	6.07
	2	400.26	27.88	52.55	5.86
	3	424.83	27.11	54.23	6.25
	7	423.07	28.87	48.98	5.98
HNO_3 Doped	0	490.57	27.86	66.92	9.15
	1	462.44	23.90	39.43	4.36

References:

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3. Y. Zhang, W. Cui, Y. Zhu, F. Zu, L. Liao, S.-T. Lee and B. Sun, *Energy Environ. Sci.*, 2014.

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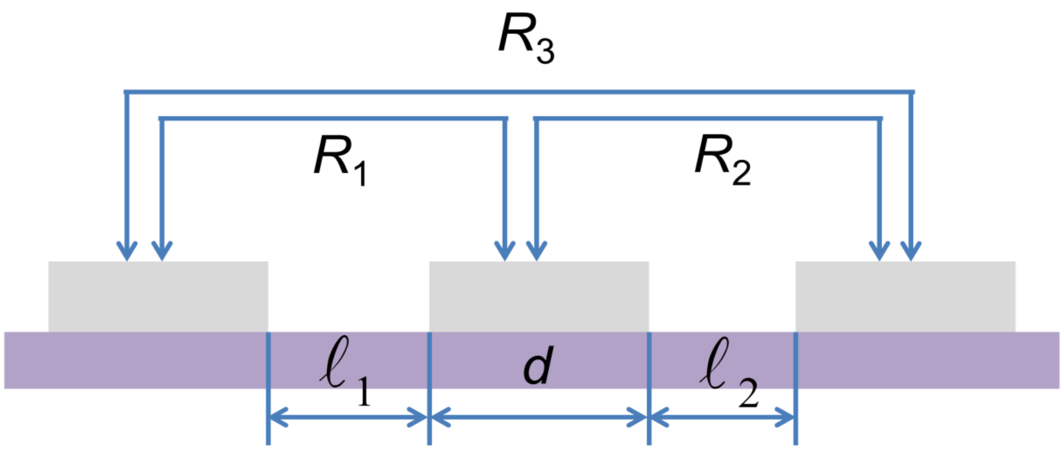

Figure. S1

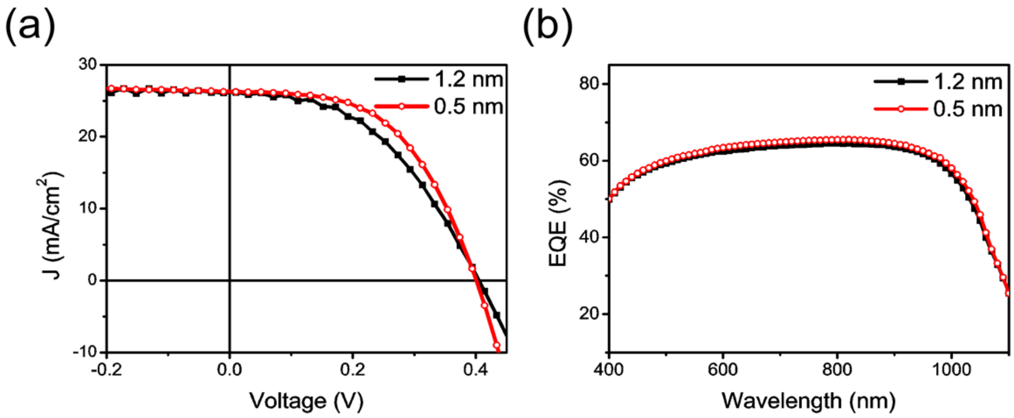

Figure S2.