Electronic Supplementary information

Enhanced broadband spectral response and energy conversion efficiency for hetero-junction solar cells with graded-sized Si quantum dots/SiC multilayers

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Photovoltaic properties of Si QDs-based solar cells with different periodicities

We have systematically studied the influences of structural parameters such as the amorphous SiC thickness and periodicity of multilayers on the cell performance containing Si QDs. It was found that both the active layer thickness and periodicity of multilayers affected the cell performance significantly. To keep the active layer thickness of the cells with various sizes of QDs means to increase the periodicity of multilayers for small-sized QDs sample (say 2 nm Si QDs), the corresponding cell exhibited the poor performance due to the strong recombination in the interface states introduced by increasing the periodicity of multilayers. As shown in Table. S1†, we prepared the Si QDs(2nm)/SiC(2nm) MLs-based with the periodicity increased to 12, which has the same active layer thickness as the Si QDs(4nm)/SiC(2nm) MLs with periodicity of 6, the corresponding V_{oc} was decreased to 388 mV while the J_{sc} was significantly decreased to 13.62 mA/cm^2, which is worse than that of Si QDs(2nm)/SiC(2nm) MLs and Si QDs(4nm)/SiC(2nm) MLs with periodicity of 6.

Table. S1 The summarized photovoltaic parameters of cell devices

	periodicity	V_{oc} (mV)	J_{sc} (mA/cm^2)	FF (%)	PCE (%)
Si(2nm)/SiC(2nm)	6	513	25.23	47.8	6.19
Si(2nm)/SiC(2nm)	12	388	13.62	31.1	1.64
Si(4nm)/SiC(2nm)	6	502	24.18	52.1	6.32

Optical absorption coefficient spectra of Si QDs/SiC multilayers

In order to compare the optical properties with the graded-sized Si QDs/SiC multilayers (MLs), periodic Si QDs/SiC MLs with Si sublayer thickness of 2nm, 4nm and 8nm were deposited on both quartz and c-Si substrates. The absorption properties of Si QDs/SiC MLs with various sizes were studied by measuring the optical transmission spectra and reflection spectra in the spectral range of 200-800 nm. The optical absorption coefficient α is calculated and given in Fig. S1(a). Based on the Tauc's plot, the optical bandgap of Si QDs/SiC MLs can be deduced from the linear fitting of $(\alpha h\nu)^{1/2} \sim h\nu$ relationship, as shown in Fig. S1(b). The deduced optical bandgap of Si QDs/SiC multilayers is 2.0, 1.5 and 1.2 eV, respectively.

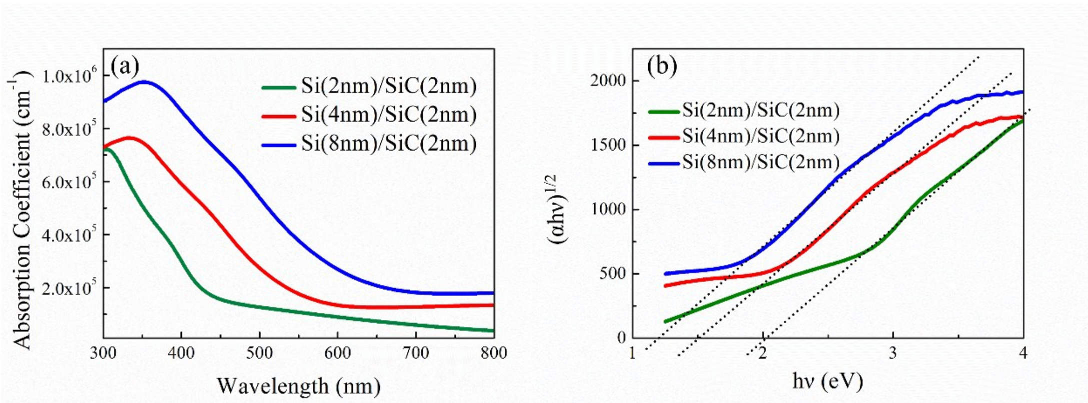

Fig. S1 (a) Optical absorption coefficient spectra of Si QDs/SiC multilayers; (b) The $(\alpha h\nu)^{1/2} \sim h\nu$ relationship.

Cross-sectional TEM images of Si QDs/SiC multilayers

Si QDs/SiC MLs with various sizes were fabricated on c-Si substrates and TEM images were measured. Figs. S2(a-c) are the high-resolution TEM images of different sized Si QDs/SiC MLs, which exhibit the formation Si QDs. The size of Si QDs is around 2.5 nm, 5.0 nm and 9.0 nm, which is well kept in the graded-sized Si QDs/SiC multilayers.

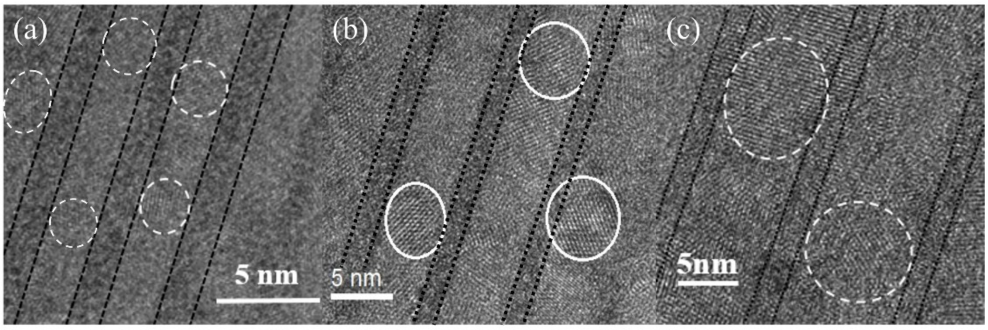

Fig. S2 The cross-sectional TEM images of (a) Si QDs(2nm)/SiC(2nm) MLs; (b) Si QDs(4nm)/SiC(2nm) MLs; (c) Si QDs(8nm)/SiC(2nm) MLs.

EQE of Si QDs/c-Si and Si QDs/Si NWs hetero-junction solar cells deposited on both n-type Si substrates and heavily-doped n-type Si substrates

In order to further understand the role of Si QDs in the present cell device, graded-sized Si QDs/SiC MLs were fabricated on heavily doped n-Si substrates (~5 mΩ•cm) to form graded-sized Si QDs/n^{++}-c-Si and Si QDs/n^{++}-Si NWs hetero-junction solar cells. The EQE results are shown in Fig. S3. The EQE is very low at the near infrared region (NIR) from 800 to 1200 nm. This is because of long wavelength light absorbed in the heavily doped substrate cannot contribute to photocurrent, due to the short minority-carrier lifetime and high recombination rate.[1] On the basis of the measured EQE spectra, J_{sc} can be estimated. The J_{sc} is about 13.89 mA/cm^2 for the flat Si QDs/n^{++}-c-Si cell and is increased to 17.35 mA/cm^2 for the graded-sized Si QDs/n^{++}-Si NWs cell. Hence, it is expected that the high spectral response in visible light region can be attributed to the contribution of graded-sized Si QDs/SiC MLs.

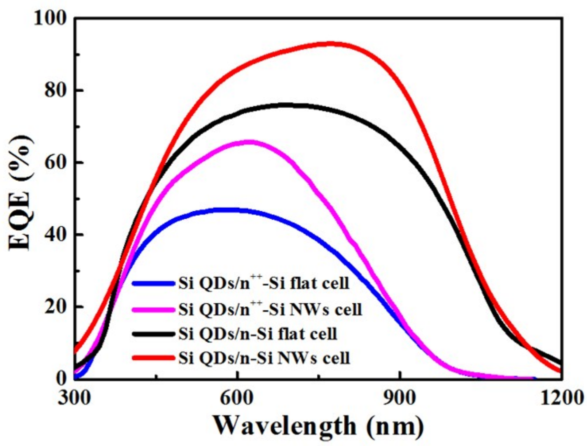

Fig. S1 External quantum efficiency of graded-sized Si QDs/c-Si and graded-sized Si QDs/Si NWs hetero-junction solar cells deposited on both n-type Si substrates and heavily-doped n-type Si substrates

References

1 M. S. Tyagi and R. Van Overstraeten, *Solid-State Electron.*, 1983, **26**, 577-597.