Area 6: Advanced Concepts and New Emerging Materials for Future PV.

SURFACE AND ENERGY BAND ENGINEERING OF ENVIROMENTALLY FRIENDLY QUANTUM DOTS FOR MULTIPLE EXCITONS SOLAR CELLS

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Although the majority of the photovoltaic market is based on silicon, silicon still presents a major limitation due to its indirect band gap which results in an overall weak light absorption and device thicknesses in the order of hundred micrometers. Nanostructuring and alloying silicon at quantum confinement size (<10 nm) could in principle solve this problem by i) engineering silicon bandgap by alloying and ii) creating a large surface/bulk ratio that due to the quantum confined regime that can allow a narrower energy gap and even trigger a direct band gap. Figure 1 illustrates the tuning of the silicon energy band gap through the surface functionalization (Fig.1a) and alloying at quantum confinement sizes (Fig.1b.), respectively. Enhanced absorption due to direct transitions will boost new physical phenomena such as carrier multiplications (CM). CM can significantly enhance solar cell efficiency (>50%) whereby carrier generation is improved through impact ionization (i.e. inverse Auger recombination) at quantum confinement. Significant improvements in term of solar cell efficiency are therefore possible through the control of alloying and surface properties at quantum confinement sizes; for instance the bandgap energy could be shifted to the optimum (i.e. a direct transition at 0.7 eV) giving a maximum efficiency for single junction solar cells. Here we show that it is particularly useful to reduce the large bandgap of quantum confined silicon nanocrystals (Si-ncs) and extend their absorption range by alloying with tin (SiSn-ncs) to absorb the solar spectrum below 1 eV. Due to the intrinsic synthesis difficulties for low-solubility binary alloys, the scientific challenge is to synthesize SiSn with Sn concentration high enough to modify the nature of the bandgap from indirect to direct transition. We achieved a SiSn-ncs alloy with a tin concentration of about 17% at confined size below 4 nm corresponding to direct transitions. Furthermore, while CM is more efficient under concentrated light (>500 suns), the surface engineering and all solar cell structure must be fabricated without the presence of organics to avoid degradation under illumination. Therefore in this work we used advanced plasma technologies to process and control alloying and surface engineering of nanocrystals. With this original approach, we successfully stabilize and improve optoelectronic properties of both Si-ncs and SiSn-ncs without large organic molecules that could hinder the transport of photogenerated carriers. We observed that during the process, Si-ncs gradually acquire oxygen-based termination including, with a certain degree of coverage, Si-OH groups. We underline that the correlation between the photoluminescence (PL) shift and the OH coverage, i.e. number of OH units on the Si-nc surface, follows a Langmuir-like adsorption rate. Our experimental data are rationalized by first-principles DFT calculations of the Si-ncs quasi-band structure. The calculations reproduce the experimental dependence of the wavelengths on the OH coverage and clarify the PL red-shift behavior. On the other hand, since the hoping transport is dominant the thickness of absorbing film plays a key role in nanocrystals based thin film solar cells. We have developed low angle deposition of surface engineered Si-ncs that allow us to fabricate thin film transparent solar cells. We demonstrate the impact of the solar cell performance produced from surface engineered nanocrystals with high optical quality and stability.

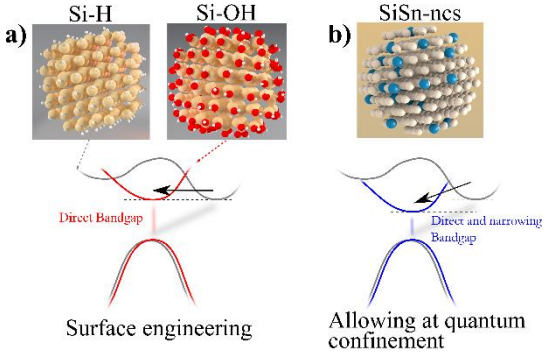

Figure 1: Illustration of the tuning of the silicon energy band gap through a) OH surface functionalization and b) alloying with tin (Sn) at quantum confinement size.