Supporting Information

Band-gap Tunable $(Cu_2Sn)_{x/3}Zn_{1-x}S$ Nanoparticles for Solar Cells

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Experimental Details

Synthesis of $(Cu_2Sn)_{x/3}Zn_{1-x}S$ ($0 \le x \le 0.75$) nanocrystals. In a typical experiment, metal chlorides (1mmol，$CuCl_2 \cdot 2H_2O$, $SnCl_2 \cdot 2H_2O$, and $ZnCl_2$ in a stoichiometric molar ratio) were dissolved in alcohol (30ml) in a beaker. Thiocarbamide (2mmol) was added into the solution and dissolved with magnetic stirring. Then the alcohol was taken out under vacuum at 50℃. The precipitate obtained was dispersed in oleylamine (10ml) and heated in a three-neck bottle at 200℃ for 10 minutes. Then the solution was cooled naturally to room temperature. Alcohol (10ml) was added gradually to the solution with magnetic stirring to precipitate the nanocrystals, followed by 2 minutes of centrifugation at 3000 rpm. The precipitate was obtained after 2 minutes of centrifugation at 3000 rpm. Washed with alcohol several times, the precipitate could disperse in toluene or hexane.

An xenon lamp ($100mW/cm^2$) was used as light source. Current-voltage curves were recorded using electrochemical analyzer. TiO_2 nanostructured films deposited on fluorine-doped SnO_2 conducting glass (FTO) using doctor blade technic formed TiO_2 electrodes. Then, the TiO_2 electrodes were sensitized by drop coating the nanocrystals. The platinized electrode was used as counter electrode. 2×10^{-3}M tetrabutylammonium perchlorate[25] dissolved in absolute alcohol and ultrapure water (volume ratio 1:1) was used as electrolyte. A 400nm cutoff filter was fitted to obtain visible light.

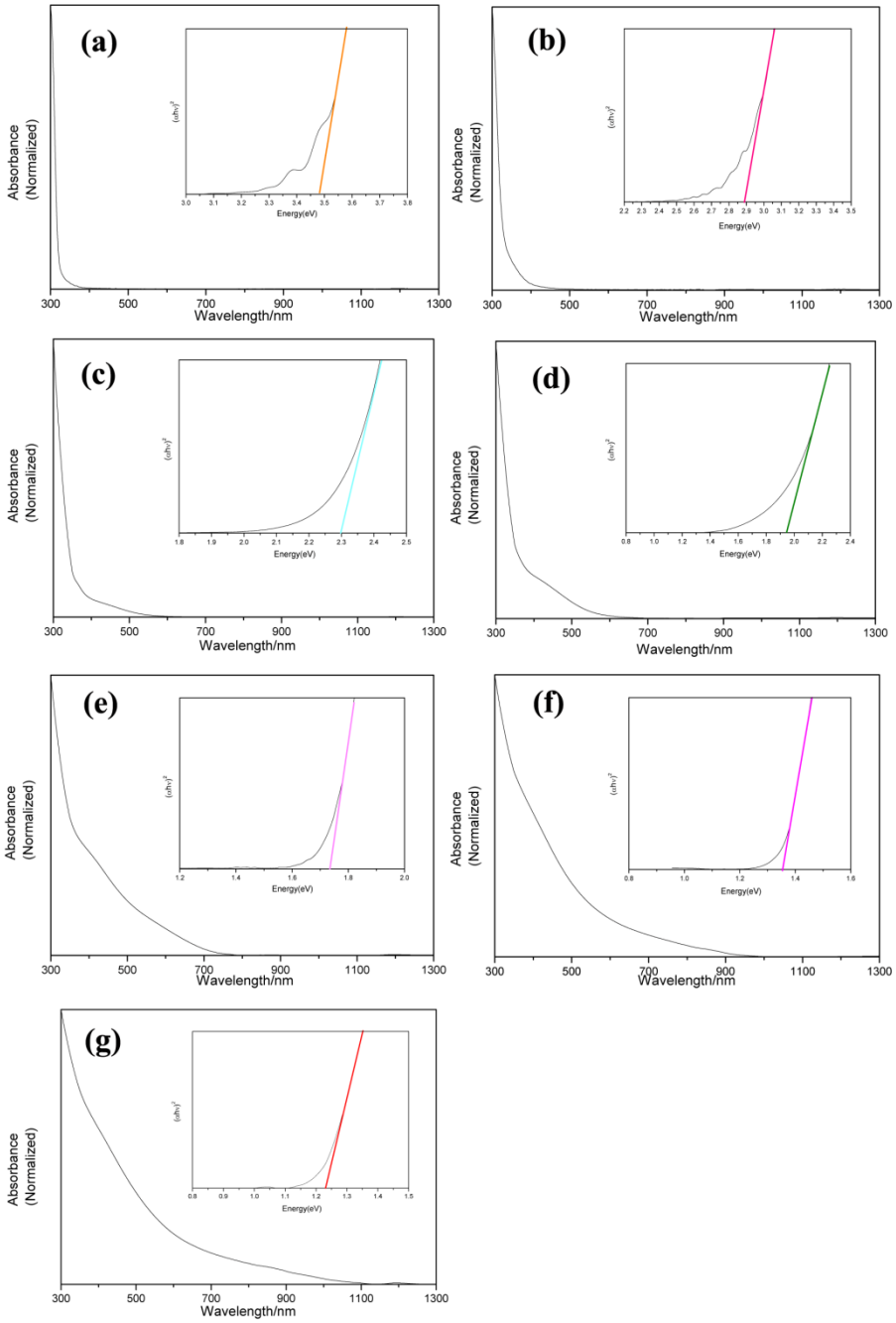

Figure S1 UV-vis absorption spectra and Color plot of $(\alpha h\nu)^2$ vs hν for nanocrystals. (a)x=0;(b)x=0.03;(c)x=0.06; (d)x=0.09; (e)x=0.24; (f)x=0.60; (g)x=0.75. Insets are Color plot of $(\alpha h\nu)^2$ vs hν. Estimated optical band gaps are obtained by the following equation, $\alpha h\nu = A(h\nu - Eg)^{m/2}$(Ref. 26), where A is a constant, α is the absorption coefficient, Eg is the band gap and m equals 1 for a direct transition. Eg could be obtained by extrapolating the linear region of plots of $(\alpha h\nu)^2$, versus energy (hν).

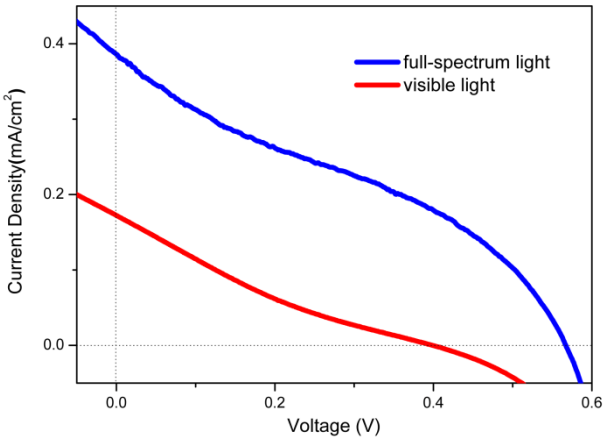

Figure S2 Current-voltage characteristics of the $(Cu_2Sn)_{0.2}Zn_{0.4}S$ (x=0.6) nanoparticles sensitized solar cell. The parameters for the solar cell under simulated sunlight are as follows: open circuit voltage of 576mV, short circuit current of 0.386 mA/cm^2, fill factor of 32.5% and a power conversion efficiency of 0.07%.

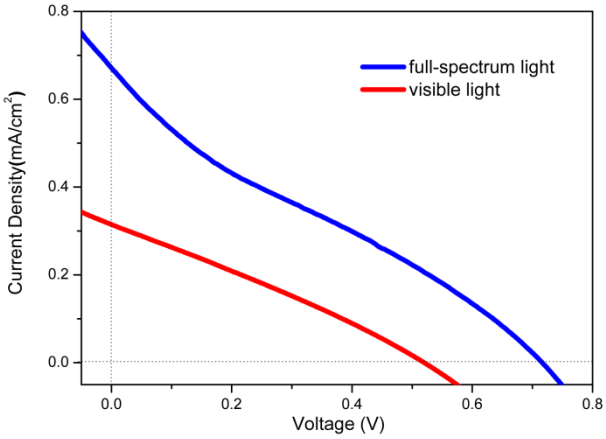

Figure S3 Current-voltage characteristics of the $(Cu_2Sn)_{0.25}Zn_{0.25}S$ (x=0.75) nanoparticles sensitized solar cell. The parameters for the solar cell under simulated sunlight are as follows: open circuit voltage of 576mV, short circuit current of 0.716 mA/cm^2, fill factor of 29.0% and a power conversion efficiency of 0.12%.

References:

25. http://www.jtbaker.com/msds/englishhtml/t0713.htm

26. J. I. Pankove, Optical Processes in Semiconductors, Prentice-Hall, New Jersey, 1971.