Supporting Information

Band-gap Tunable (Cu$_2$Sn)$_{x/3}$Zn$_{1-x}$S Nanoparticles for Solar Cells

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**Experimental Details**

Synthesis of (Cu$_{2}$Sn)$_{x/3}$Zn$_{1-x}$S ($0 \leq x \leq 0.75$) nanocrystals. In a typical experiment, metal chlorides (1 mmol, CuCl$_2$·2H$_2$O, SnCl$_2$·2H$_2$O, and ZnCl$_2$ in a stoichiometric molar ratio) were dissolved in alcohol (30 ml) in a beaker. Thiocarbamide (2 mmol) was added into the solution and dissolved with magnetic stirring. Then the alcohol was taken out under vacuum at 50°C. The precipitate obtained was dispersed in oleylamine (10 ml) and heated in a three-neck bottle at 200°C for 10 minutes. Then the solution was cooled naturally to room temperature. Alcohol (10 ml) 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 (100 mW/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 dissolved in absolute alcohol and ultrapure water (volume ratio 1:1) was used as electrolyte. A 400 nm cutoff filter was fitted to obtain visible light.
Figure S1 UV-vis absorption spectra and Color plot of \((\alpha h\nu)^2\) vs \(h\nu\) 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 \(h\nu\). Estimated optical band gaps are obtained by the following equation, \(\alpha h\nu = A(h\nu-E_g)^m/2\) (Ref. 26), where \(A\) is a constant, \(\alpha\) is the absorption coefficient, \(E_g\) is the band gap and \(m\) equals 1 for a direct transition. \(E_g\) could be obtained by extrapolating the linear region of plots of \((\alpha h\nu)^2\), versus energy \((h\nu)\).
Figure S2 Current-voltage characteristics of the (Cu$_2$Sn)$_{0.6}$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$_2$Sn)$_{0.75}$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: