Electronic Supplementary Material (ESI) for Nanoscale

SUPPORTING INFORMATION

Controlled Growth of ZnO/$Zn_{1-x}Pb_xSe$ Core-shell Nanowires and their Interfacial Electronic Energy Alignment

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***J–V* characteristics of ZnO/$Zn_{1-x}Pb_xSe$ Core-shell Nanowires:**

The modulus of the ZnO/$Zn_{1-x}Pb_xSe$ core-shell NWs based sensitizing solar cells was illustrated in Fig. S1(a). Under illuminations, e^--h^+ pairs are generated in the $Zn_{1-x}Pb_xSe$ shells, while the excited electrons are transported to the conduction band of ZnO NWs, and drifted to the FTO electrode. The electrons donated by the redox species of the electrolyte compensate the lost electrons. The simultaneously generated sulfur, S and S^{2-} leads to the formation of polysulfide. The S_2^{2-} then obtains electrons at the counter electrode and regenerate oxidized sulfide (S^{2-}). The electrons transfer process of the redox couple should be fast and their redox potential should be sufficiently negative to provide electrons to the $Zn_{1-x}Pb_xSe$ film continuously.

The *J–V* characteristics obtained under simulated illumination of 100mWcm^{-2} for the devices with sensitizer of ZnSe, $Zn_{0.9}Pb_{0.1}Se$, $Zn_{0.64}Pb_{0.36}Se$ and $Zn_{0.34}Pb_{0.66}Se$ has been illustrated in Fig. S1(b). The detailed parameters of V_{oc}, J_{sc}, series resistance (R_s) and shunt resistance (R_{sh}) are shown in Table S1.

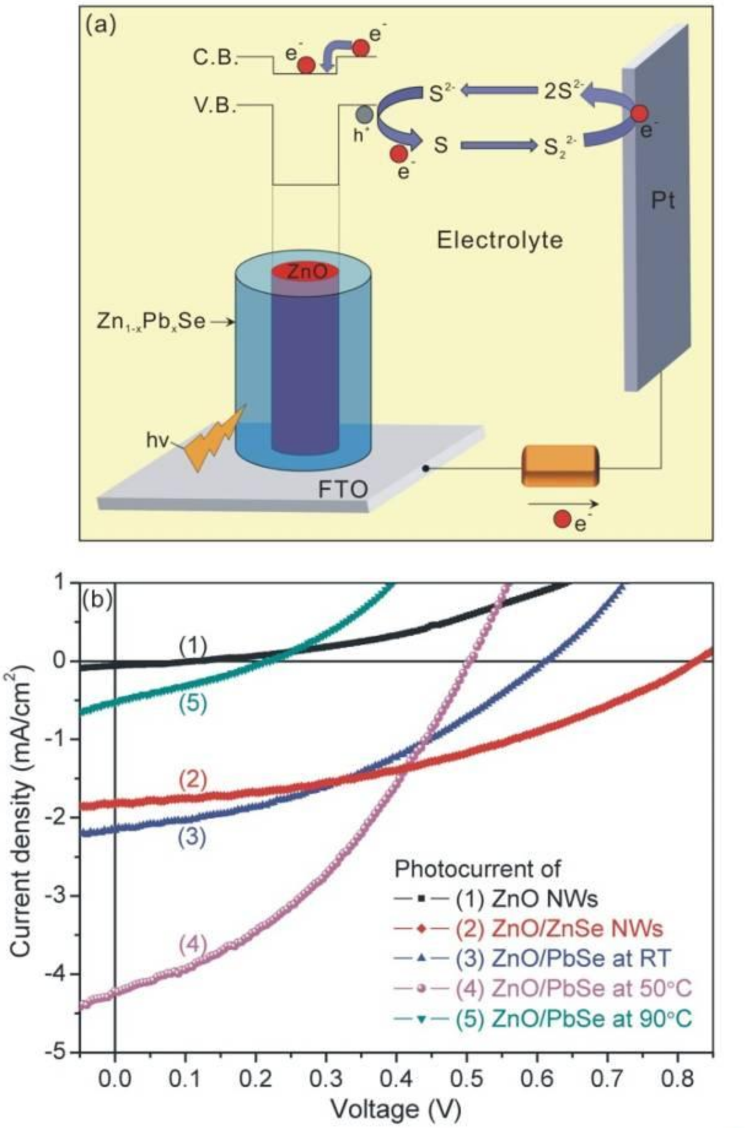

Figure S1: Construction and mechanism of core-shell NWs based solar cell device. (b) *J–V* characteristics for bare ZnO NWs, ZnO/ZnSe NWs and $ZnO/Zn_{1-x}Pb_xSe$ core-shell NWs.

Resistance study of $ZnO/Zn_{1-x}Pb_xSe$ NWs:

The resistance values of R_s and R_{sh} can be approximately estimated as the inverse of the slopes of the *J-V* curve at V_{oc} and J_{sc}, respectively.[1-4] Table S1 lists the parameters of J_{sc}, V_{oc}, R_s, and R_{sh} of the solar cells based on $ZnO/Zn_{1-x}Pb_xSe$ NWs.

J_{sc} and V_{oc} of the solar cells are dependent on the R_{sh} and R_s of the devices.[5] The larger R_{sh} contributes to the higher V_{oc}, while the smaller R_s contribute to the higher J_{sc}. It can be seen that the R_{sh} of the ZnO/ZnSe device are much higher than those of the others, implying that these devices would have the largest V_{oc}. For the $ZnO/Zn_{1-x}Pb_xSe$ devices with band

II alignment, ZnO/$Zn_{0.64}Pb_{0.36}Se$ core-shell NWs has the smallest R_s, which leads to its highest J_{sc}. The device based on ZnO/$Zn_{0.34}Pb_{0.66}Se$ core-shell NWs have a band I alignment, forming a barrier that obstructs the charge transfer at the interface and results in an ultra-low J_{sc}.

Table S1: Series resistance (R_s) and shunt resistance (R_{sh}), J_{sc} and V_{oc} of the solar cells based on various ZnO/$Zn_{1-x}Pb_xSe$ core-shell structures.

Core-shell NWs	ZnO/ZnSe	ZnO/$Zn_{0.9}Pb_{0.1}Se$	ZnO/$Zn_{0.64}Pb_{0.36}Se$	ZnO/$Zn_{0.34}Pb_{0.66}Se$
J_{sc}	1.82	2.17	4.22	0.52
V_{oc}	0.83	0.61	0.50	0.22
R_s	188.7	150.6	63.6	315.3
R_{sh}	1578.8	772.3	321.4	431.4

J_{sc} of a photovoltaic cell device under illuminations:

The *J-V* characteristics of the photochemical solar cells show that the short circuit current density gradually increases with the elapsed time until reaching stable values. During the illumination heating process, more excited electrons pass through the ZnO/$Zn_{1-x}Pb_xSe$ interface which results in increasing electron-transfer to the photoanode as well as enhancing photocurrent. After illumination for 180s, the J_{sc} turns to a constant value and becomes stable.

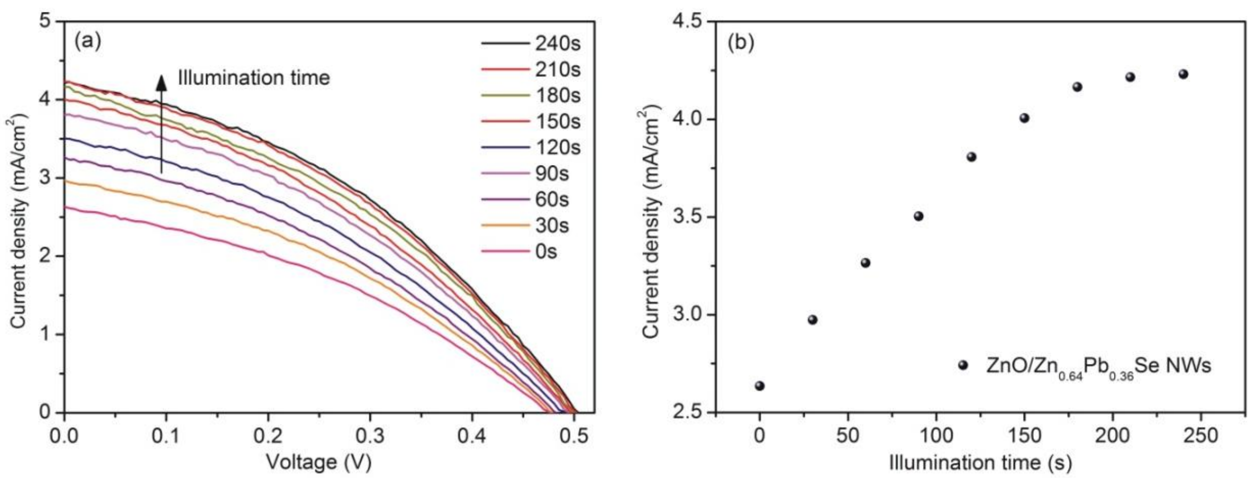

Figure S2: (a) *J–V* characteristics for ZnO/$Zn_{0.64}Pb_{0.36}Se$ core-shell NWs. (b) Short circuit current density (J_{sc}) changes with illumination time.

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Reference:

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