Supporting Information

Enhanced performance of the Sb_2Se_3 thin-film solar cell by an organic molecule induced crystallization and a suppression of the interface recombination

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1. Experiment and measurement

Sb_2Se_3 (99.999%) were purchased from Sigma. C_{60} (sublimed grade, ≥99.0%), Alq_3 (sublimed grade, ≥99.0%), and NPB (sublimed grade, ≥99.0%) were purchased from Han Feng. Solar cells were fabricated by the vacuum thermal evaporation with a base pressure of 2.0×10^{-4} Pa on commercially patterned indium tin oxide (ITO) coated glass with a sheet resistance of ~15 Ω cm^{-2}. Substrates were ultrasonically washed in acetone, alcohol, and deionized water in sequence, and then dried by a flow of nitrogen gas. Substrates were subsequently baked the in air at 200 °C for 20 min. Next, NPB and Sb_2Se_3 were successively deposited by vacuum thermal evaporation, and the substrate

was kept at room temperature. Then, the vacuum was broken and the substrate was transferred to a vacuum tube furnace with two temperature zones to anneal in the atmosphere of Se at 280 °C for 30 min, and was naturally cooled down to room temperature. During annealing treatment the source of Se was kept at 210 °C, and a mixture of the argon (Ar) and hydrogen (H_2) gas (v:v = 10:1, 99.999%) was introduced to the tube with a flux of 30 sccm, and the pressure in the tube was ~35 Pa. After that, C_{60} and Alq_3 were successively deposited by the vacuum thermal evaporation. Finally, the substrate was transferred to another chamber without breaking the vacuum, in which the Al electrode was deposited. A stainless shadow mask was used to define the device profile (1.5×5.0 mm^2). The film thickness was monitored by a quartz crystal microbalance. The deposition rates were ~0.1 nm s^{-1} for the NPB, Sb_2Se_3, C_{60} and Alq_3, and ~2.0 nm s^{-1} for the Al electrode.

X-ray diffraction (XRD) was performed on a Shimadzu XRD-6100. Surface and cross-sectional images of the Sb_2Se_3 film were measured on a Bruker scanning electron microscopy (SEM). Absorption spectra were measured on a Shimadzu UV3600 spectrophotometer. Raman spectra were obtain on a Renishaw inVia confocal Raman spectrometer with a 532 nm laser as excitation source. TA spectra (Time-Tech Spectra, Femto-TA100) were measured using previously described methods.[1] The full-width at half-maximum of the pump pulse was ~ 80 fs, and the time resolution was 50 fs. All the TA spectra were measured with a 920-nm pump pulse. The pump beam was focused to a diameter of ~300 μm. The sample was moved with a velocity of 0.3 mm s^{-1} during the TA measurements. The current density–voltage (*J–V*) measurements were performed on a Keithley 2611A source meter. The photovoltaic response was obtained under AM1.5 illumination from a Zolix Sirius-SS150A solar simulator (class AAA) at a power of 100 mW cm^{-2}. The illumination intensity on the cell was adjusted by a standard calibrated Si solar cell. External quantum efficiency (EQE) was measured on a Zolix SCS100 analyzer. The capacitance measurements were performed on an Agilent B1500A semiconductor device analyzer in the dark, where an alternating current voltage of 30 mV was applied.

[1]J. Liu, J. Leng, K. Wu, J. Zhang and S. Jin, Journal of the American Chemical Society **139**, 1432-1435 (2017).

2. Extraction of the device parameters from the *J–V* characteristics

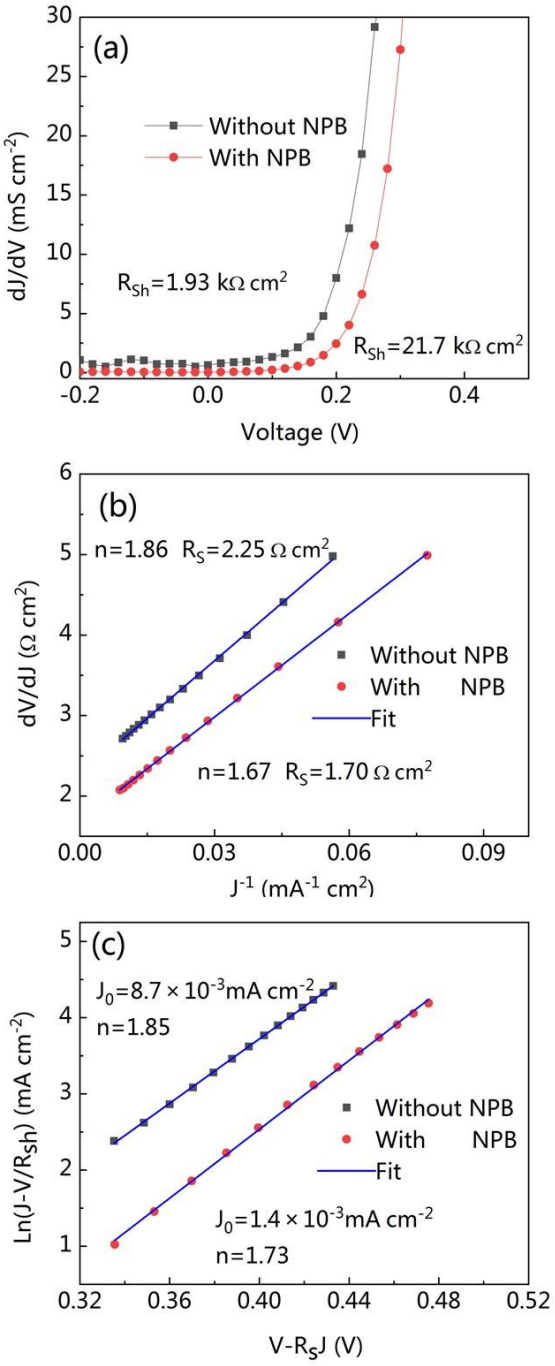

Figure S1 (a) d*J*/d*V* *vs*. *V*, (b) d*V*/d*J* *vs*. J^{-1}, and (c) ln(*J*−*V*/ R_{sh}) *vs*. (*V*−*JR*$_s$) curves calculated from the *J–V* characteristics in the dark. The points are experimental data, and the solid bule lines are the best fits in the (b) and (c).

The *J*–*V* characteristics of the device can be described by

$$J = J_0 \exp(\frac{V - JR_s}{nk_BT}) + \frac{V}{R_{sh}} - J_L , \qquad (2)$$

where, J_0 is the reverse saturated current density, n is the ideality factor, k_B is the Boltzmann constant, R_s is the series resistance, R_{sh} is the shunt resistance, T is the absolute temperature, and J_L is the photocurrent density. J_L is equal to 0 in the dark. R_{sh} can be obtained from the flat zone on the curve of dJ/dV *vs.* V. R_s and n can be obtained from the intercept and the slope of the dV/dJ *vs.* J^{-1} curves, respectively. J_0 and n can be obtained from the intercept and slope of the ln(J–V/R_{sh}) *vs.* (V–JR_s) curve.

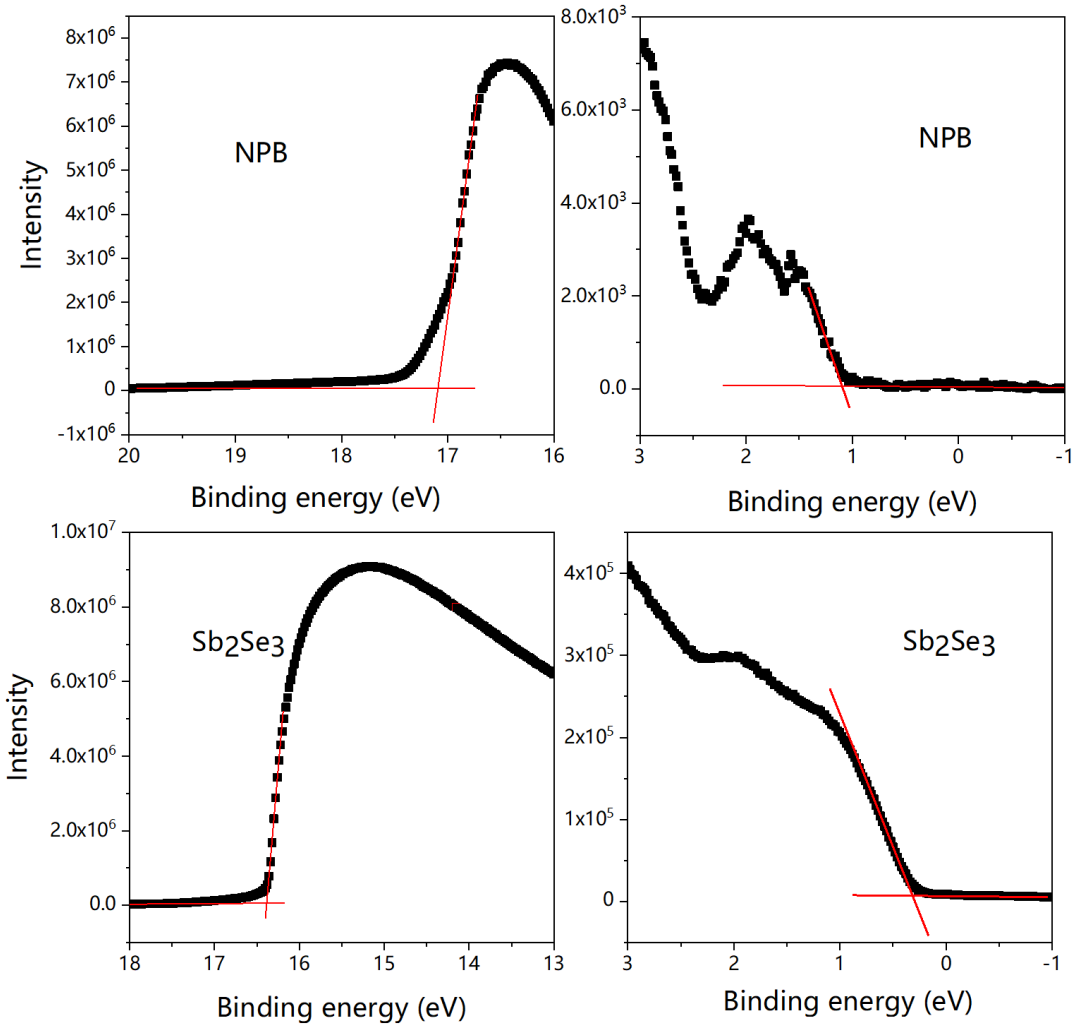

Figure S2 UPS of the NPB and Sb_2Se_3 films.