Electronic Supporting Information

Novel MoS_2-based hybrid film as the back electrode for high-performance thin film solar cells

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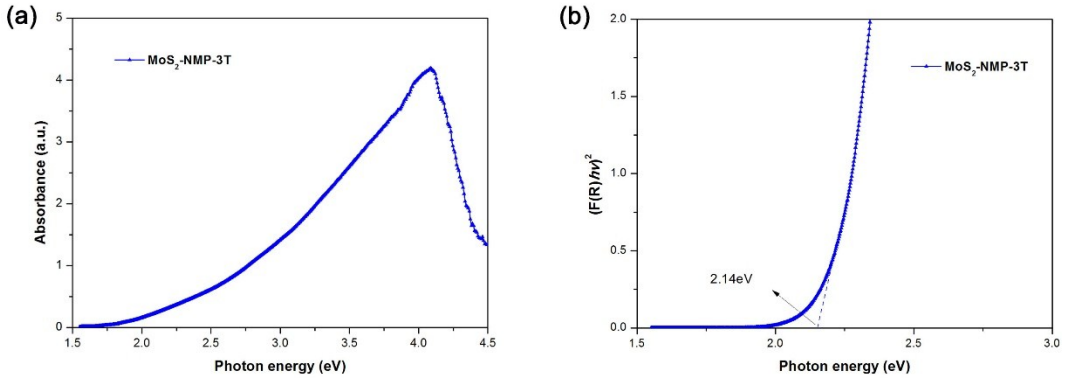

Figure S1. (a) The UV-Vis absorption spectrum of MoS_2-NMP films (MoS_2-NMP-3T) which was prepared by spin-coating MoS_2-NMP solution three times; (b) plots of $(F(R)\,h\nu)^2$ versus photon energy ($h\nu$) for estimation of the band gaps of MoS_2-NMP films according to the direct band gap (because single layer MoS_2 is a direct band gap semiconductor)

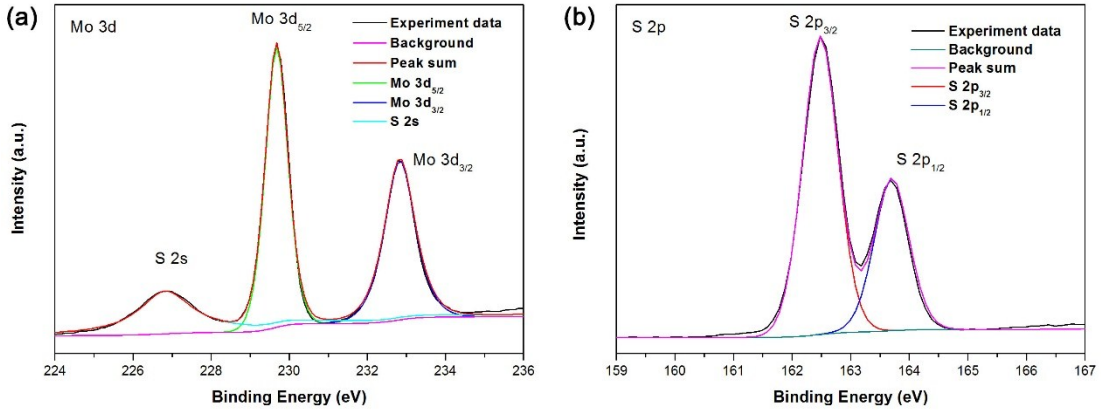

Figure S2. XPS spectra of (a) Mo 3d and (b) S 2p for pure MoS_2 powder.

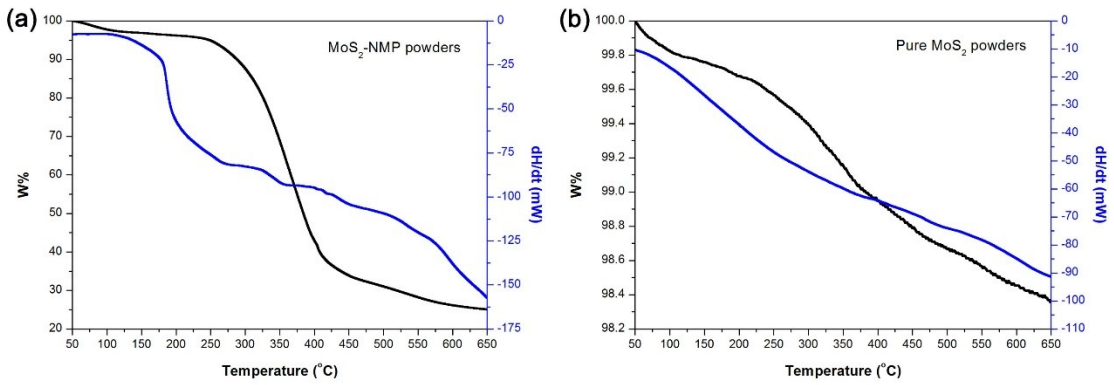

Figure S3. (a) The TG and DSC curves of MoS_2-NMP powder. (b) the TG and DSC curves of raw materials MoS_2.

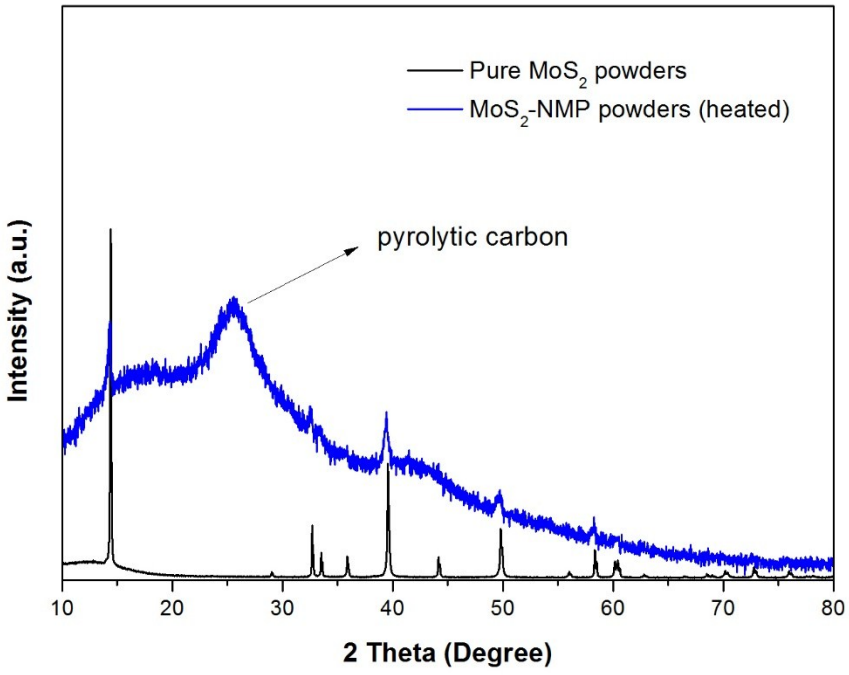

Figure S4. The powder X-ray diffraction pattern of MoS_2-NMP after the thermal treatment at 430℃ for 40 min in an Ar-filled golvebox.

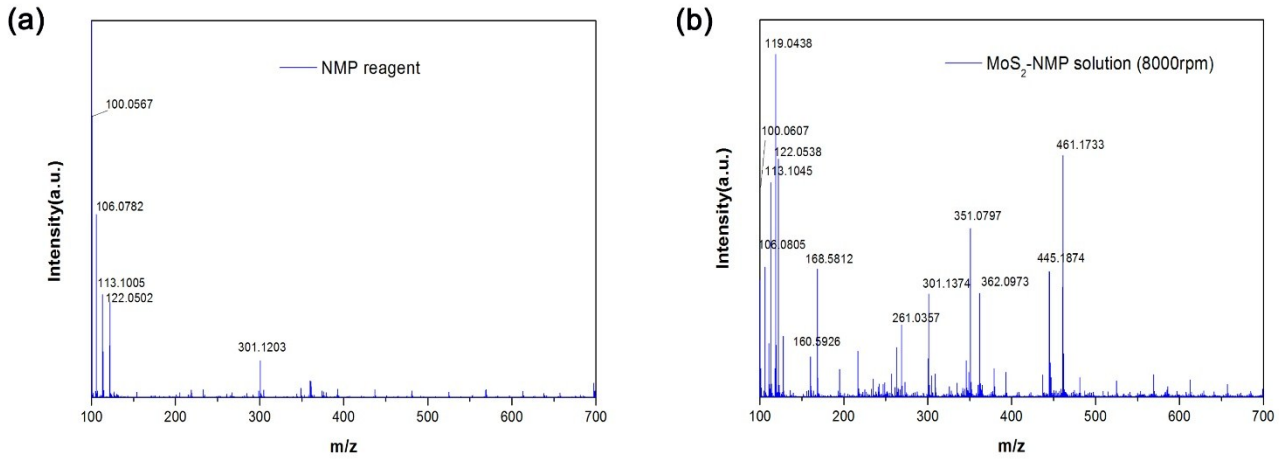

Figure S5. The mass spectra of pure NMP reagent (a) and MoS_2-NMP solution (b).

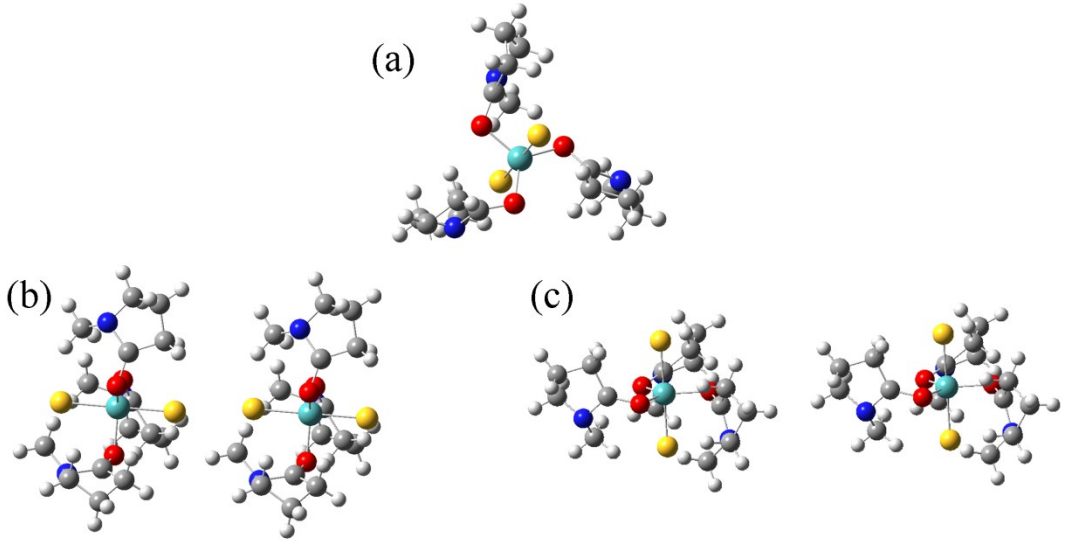

Figure S6. Three proposed models for the structure of $MoS_2(NMP)_3$. (a) one molecule of $MoS_2(NMP)_3$; (b) the serial stacking of two $MoS_2(NMP)_3$ molecules; (c) the parallel stacking of two $MoS_2(NMP)_3$ molecules.

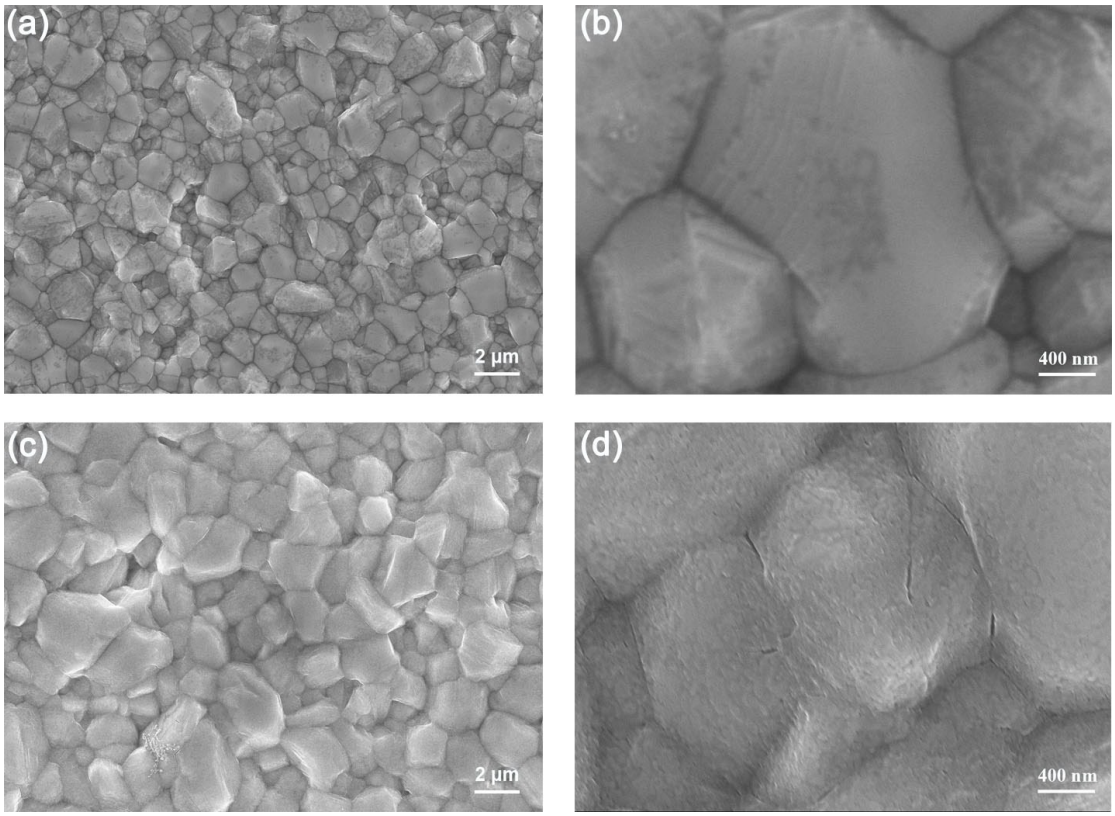

Figure S7. (a) Low and (b) high magnification SEM images of the surface for traditional CdTe solar cell with a FTO/CdS/CdTe/Cu/Au configuration; (c) Low and (d) high magnification SEM images of the surface when adopting MoS_2-based thin film as the back contact.

The calculation detail for the work function of MoS_2-based thin film:

$$\Phi_{MoS_2-NMP} - \Phi_{tip} = -eV_{CPD2} = 0.13eV$$

$$\Phi_{Au} - \Phi_{tip} = -eV_{CPD1} = 0.03eV$$

$$\Phi_{MoS_2-NMP} - \Phi_{Au} = -e(V_{CPD2} - V_{CPD2}) = 0.1eV$$

$$\Phi_{Au} = 5.32eV$$

$$\Phi_{MoS_2-NMP} = 5.42eV$$