Supporting Information

Vertically Aligned 1T-phase $PtSe_2$ on Flexible Carbon Cloth for Efficient and Stable Hydrogen Evolution Reaction

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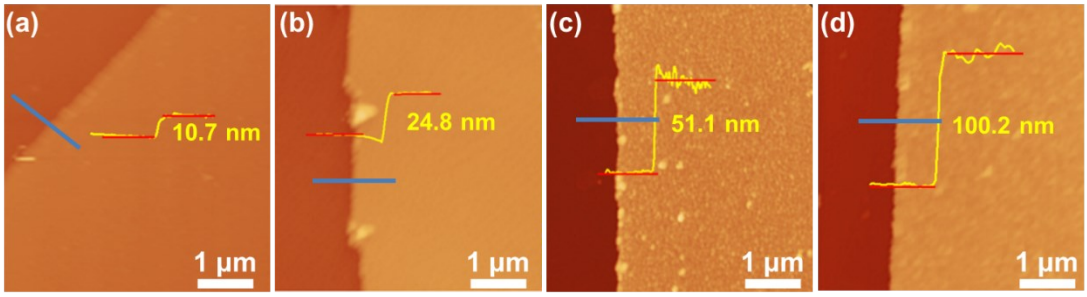

Fig. S1 AFM images and corresponding height profiles for $PtSe_2$ samples on Si substrate, and the growing procedures of them are same with that of (a) $PtSe_2$-1, (b) $PtSe_2$-2, (c) $PtSe_2$-3 and (d) $PtSe_2$-4, respectively.

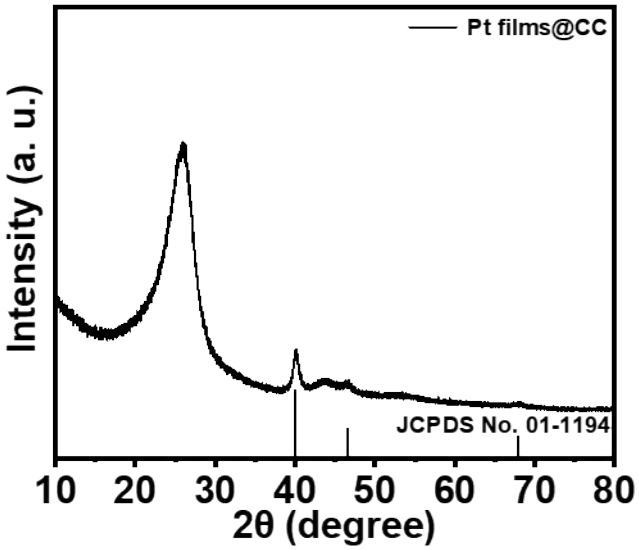

Fig. S2 XRD characterization of Pt films sputtered on the substrate of bare CC.

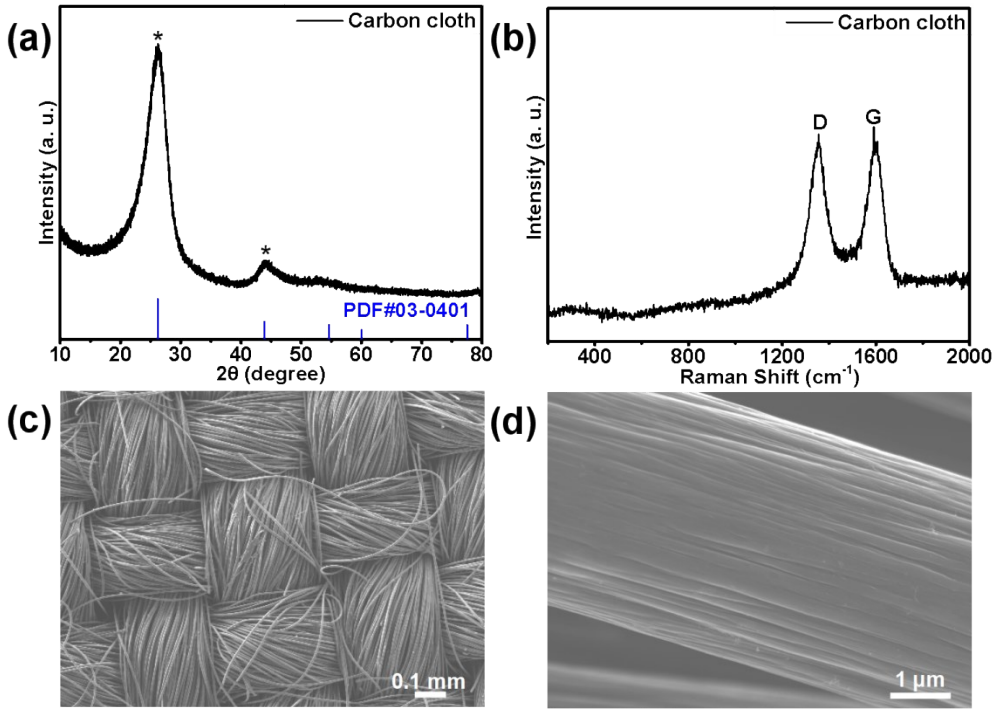

Fig. S3 (a) XRD patterns and (b) Raman spectra of the bare carbon cloth; (c, d) SEM images of the bare carbon cloth at different magnifications used for the fabrication of functional electrodes.

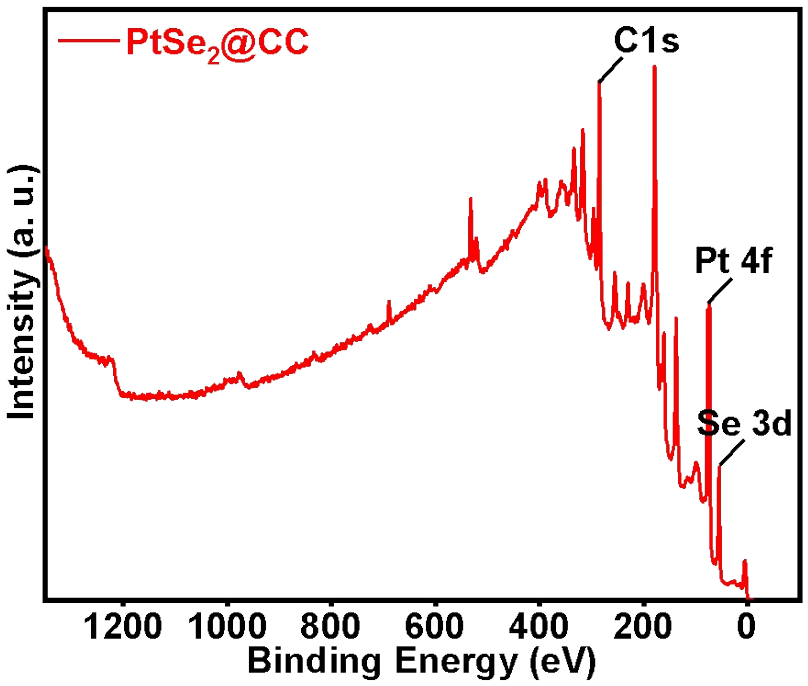

Fig. S4 Wide-scan XPS spectrum of $PtSe_2$@CC.

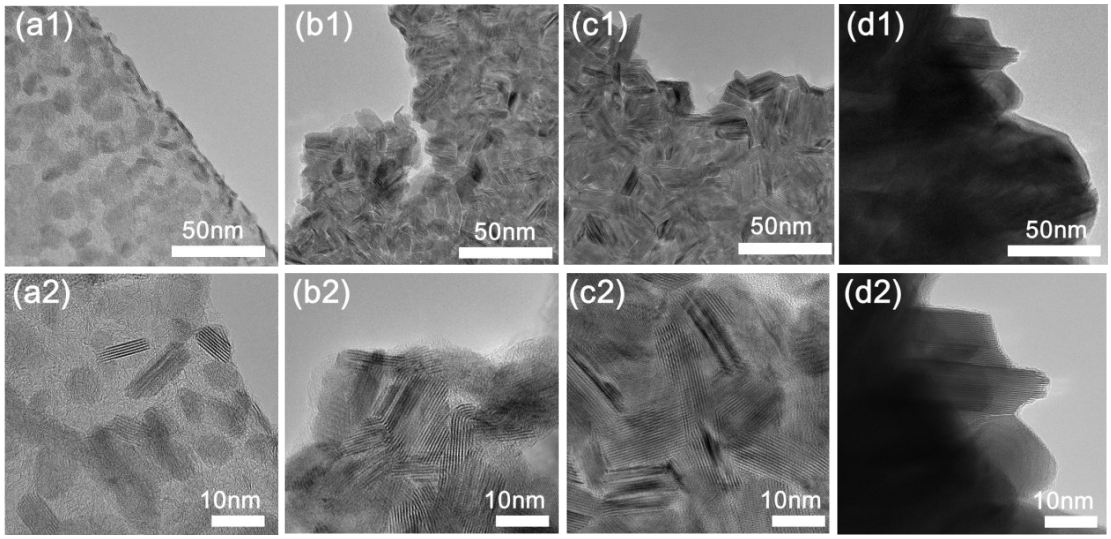

Fig. S5 (a1-a2), (b1-b2), (c1-c2) and (d1-d2) are the low and high-resolution images of $PtSe_2$ samples ($PtSe_2$@CC-1, $PtSe_2$@CC-2, $PtSe_2$@CC-3 and $PtSe_2$@CC-4, respectively.)

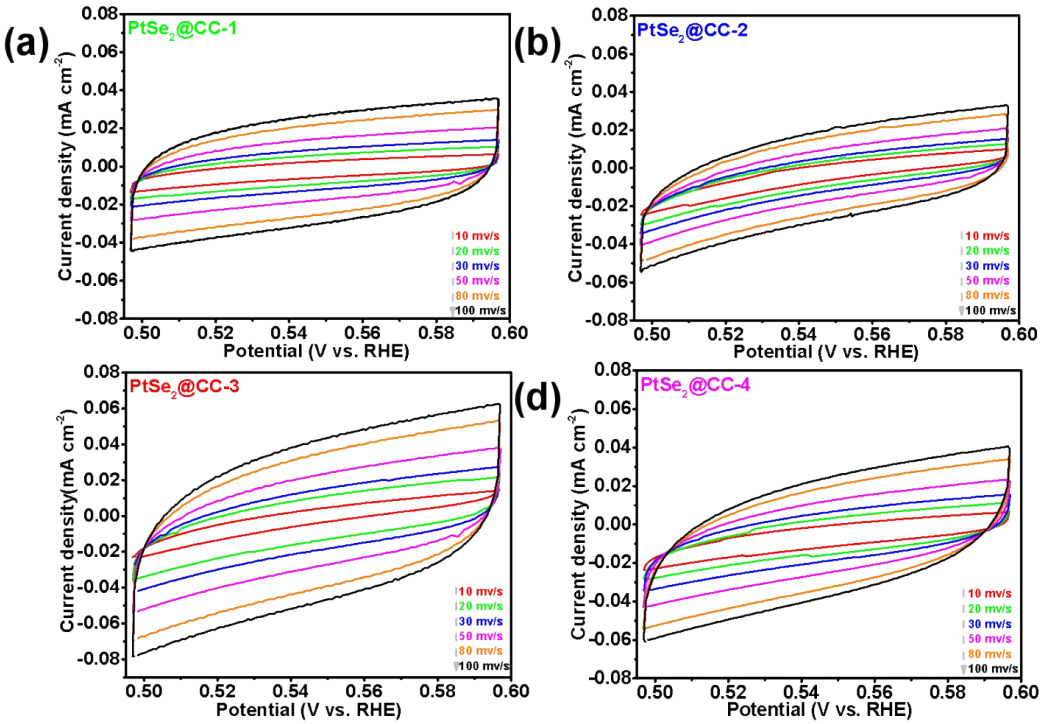

Fig. S6 Electrochemical cyclic voltammetry curves of as-grown $PtSe_2$@CC samples with different $PtSe_2$ thickness. (a) $PtSe_2$@CC-1, ~10.7 nm; (b) $PtSe_2$@CC-2, ~24.8 nm; (c) $PtSe_2$@CC-3, ~51.1 nm and (d) $PtSe_2$@CC-4, ~100.2 nm. The scan rates are in the ranges from 10 mV/s to 100 mV/s.

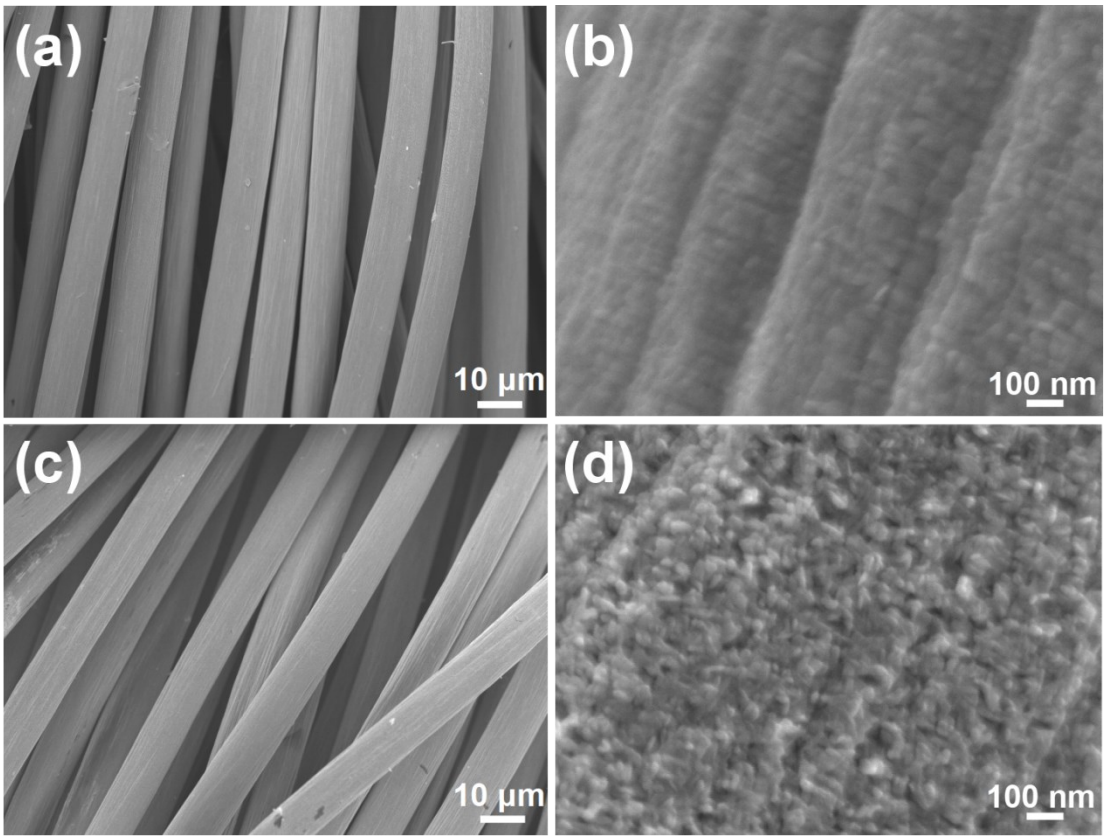

Fig. S7 The SEM results for conducting chronoamperometry measurement for 30 h of $PtSe_2$@CC-3. the morphology of $PtSe_2$@CC-3 was characterized before (a)-(b) and (c)-(d) after 30 h.

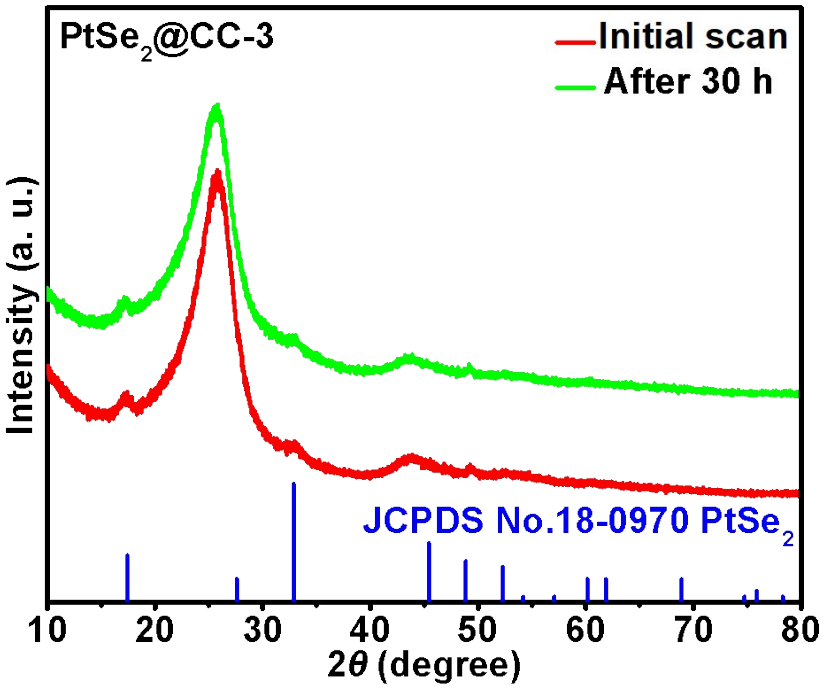

Fig. S8 The XRD results that conducted chronoamperometry measurement before and after 30 h of $PtSe_2$@CC-3.

Table S1 Comparisons of HER performances of TMDCs-based catalysts on the various flexible carbon substrate, such as carbon fiber (CF), carbon cloth (CC) and carbon fiber paper (CFP).

catalyst	Substrate	η_{10} (mV)	Tafel slope (mV dec^{-1})	Method	Ref.
WS_2	CC	175	98	hydrothermal	[1]
Ni-doped MoS_2	CC	136	72	hydrothermal	[2]
$MoSe_2$	CF	186	88	hydrothermal	[3]
Co-Doped VSe_2	CC	180	63	hydrothermal	[4]
ReS_2	CC	171	100	hydrothermal	[5]
MoS_2/VS_2	CFP	200	95.2	CVD	[6]
Co-doped $MoSe_2$	CC	210	91	solvothermal	[7]
Ni-doped $MoSe_2$	CC	226	95	solvothermal	
$PtSe_2$@ CC-3	**CC**	**177**	**67**	**CVD**	**This work**

The treatment of the carbon cloth substrate:

Before Pt sputtering, the carbon cloth is treated as the following process: The carbon cloth substrates were first soaked in concentrated nitric acid (65%) at room temperature for overnight to improve their hydrophilicity as well as remove impurities from the surface of the carbon cloth. Afterwards, the carbon cloth was rinsed repeatedly with deionized water and alcohol, and then dried under vacuum at 60 ℃ for 6 h.

Theoretical calculations:

In the adsorption structures, the slab was separated by a 2 nm vacuum space. The 1T-edge was simulated using a 2×4×4 slab model, with x direction and the vertical direction of the midline of y and z vertors being continuous while the midline direction of y and z direction separated by vacuum slabs. A 5×5×1 k-mesh was used to sample the first Brillouin zone of unit cell on 2L-$PtSe_2$. All atoms were relaxed until the residual force for each atom is less than 0.03 eV $Å^{-1}$. The hydrogen binding energy (E_b) can be obtained from the following equation:

$$E_b = E_{total} - E_H - E_{slab}$$

Where E_{total}, E_H and E_{slab} are the energy of H adsorbed on the slab, the energy of H atom, and the energy of the slab before H adsorption.

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