Electronic supplementary information

Mo₂C coated with Ni nanoparticles as cathode catalyst towards efficient hydrogen evolution reaction: an experimental and computational investigation

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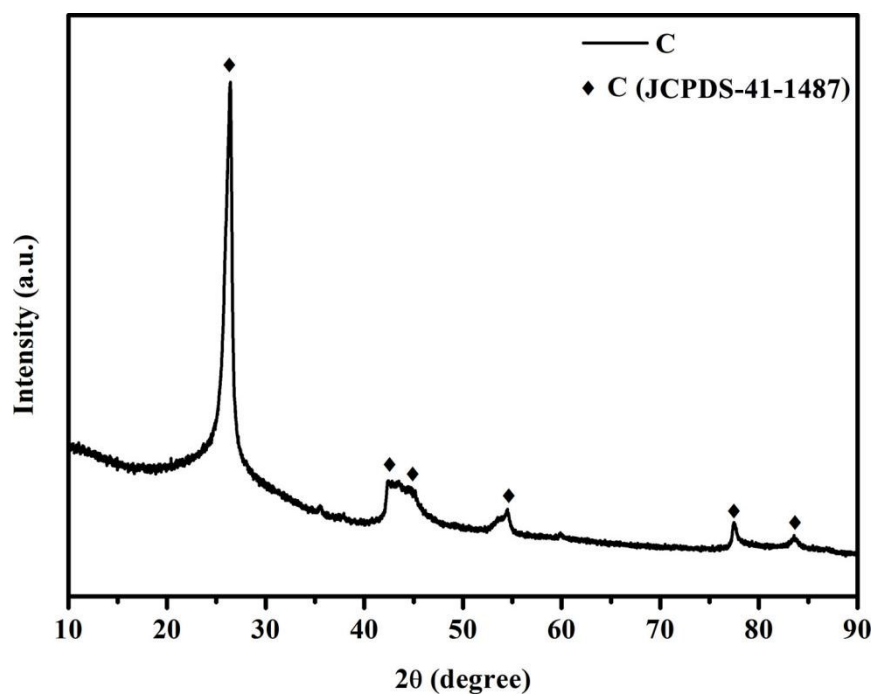
Fig. S1 XRD pattern of fabricated C material.
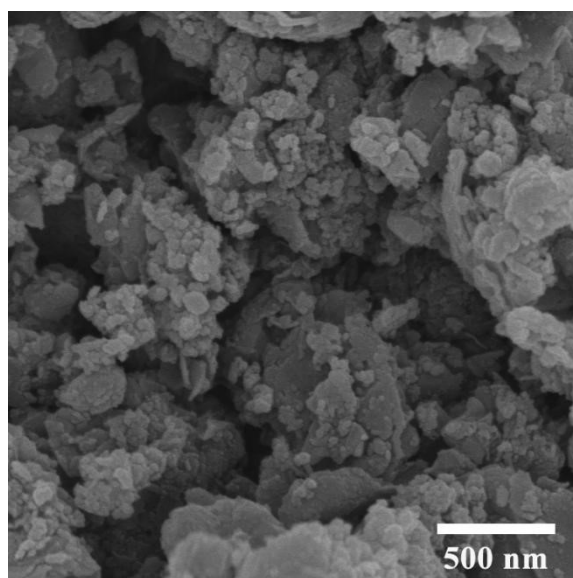
Fig. S2 SEM image of synthesized alkynyl carbon.

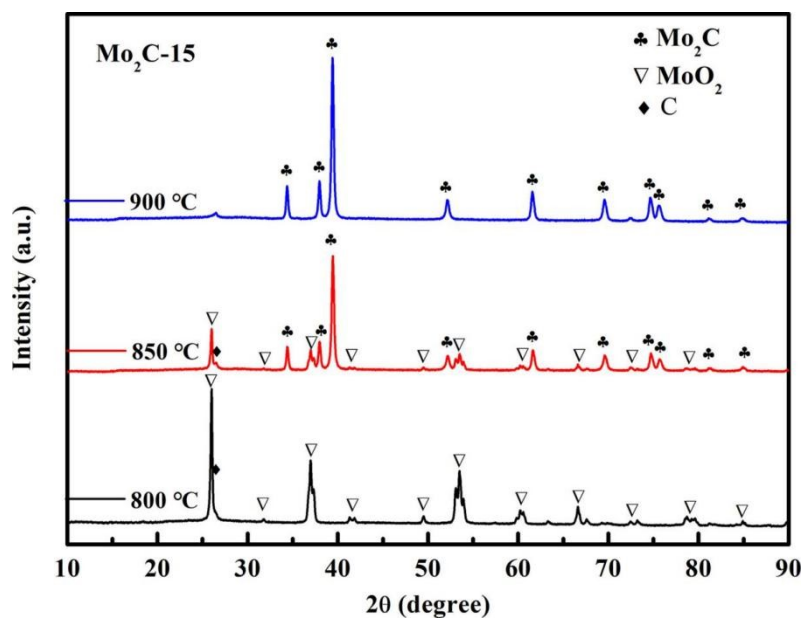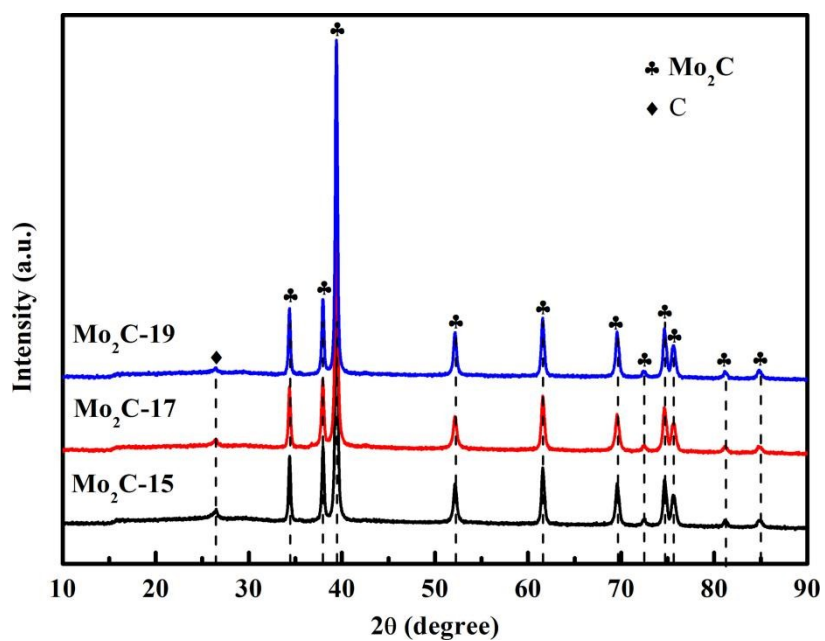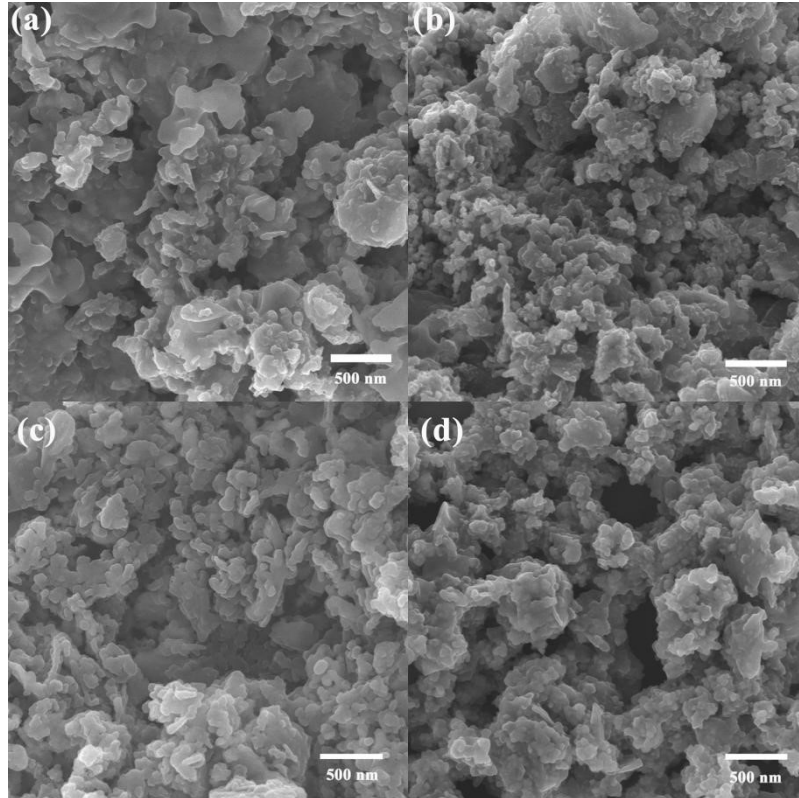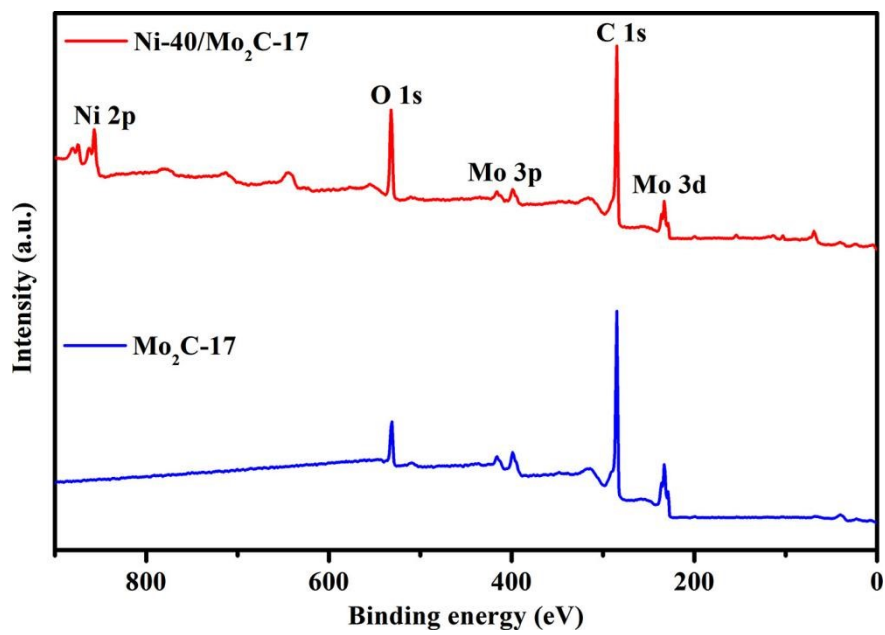**Fig. S3** XRD patterns of Mo$_2$C-15 prepared at different temperature.

Fig. S4 XRD patterns of Mo$_2$C-15, Mo$_2$C-17, Mo$_2$C-19 samples.

Fig. S5 (a) SEM image of Ni-30/Mo$_2$C-17. (b) SEM image of Ni-50/Mo$_2$C-17. (c) SEM image of Mo$_2$C-17. (d) SEM image of Ni-40/C.

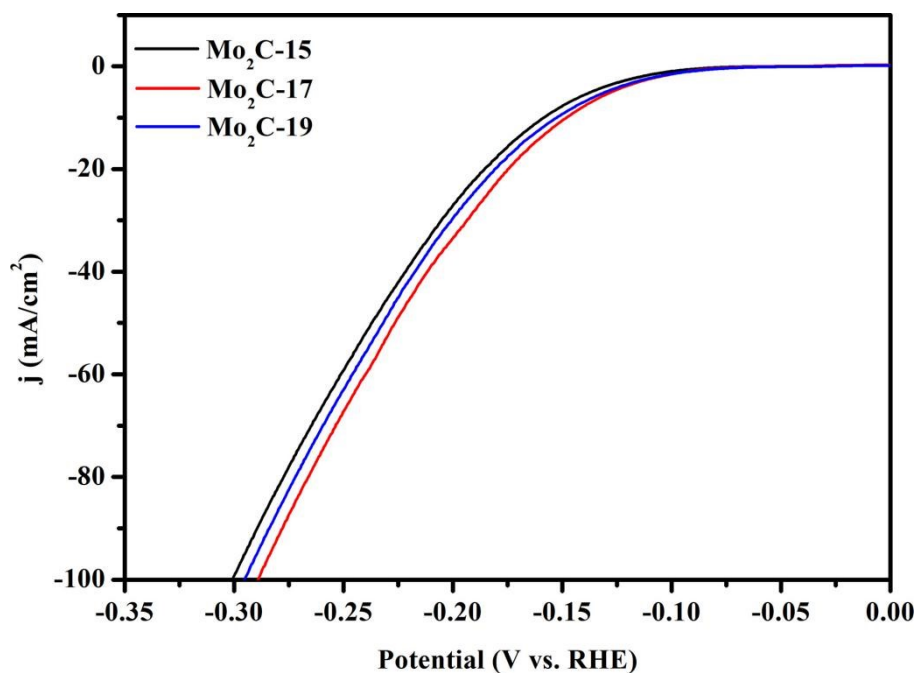**Fig. S6** XPS full scans of Mo$_2$C-17 and Ni-40/Mo$_2$C-17.

Fig. S7 Polarization curves of Mo_2C prepared by molybdenum precursor with different content.
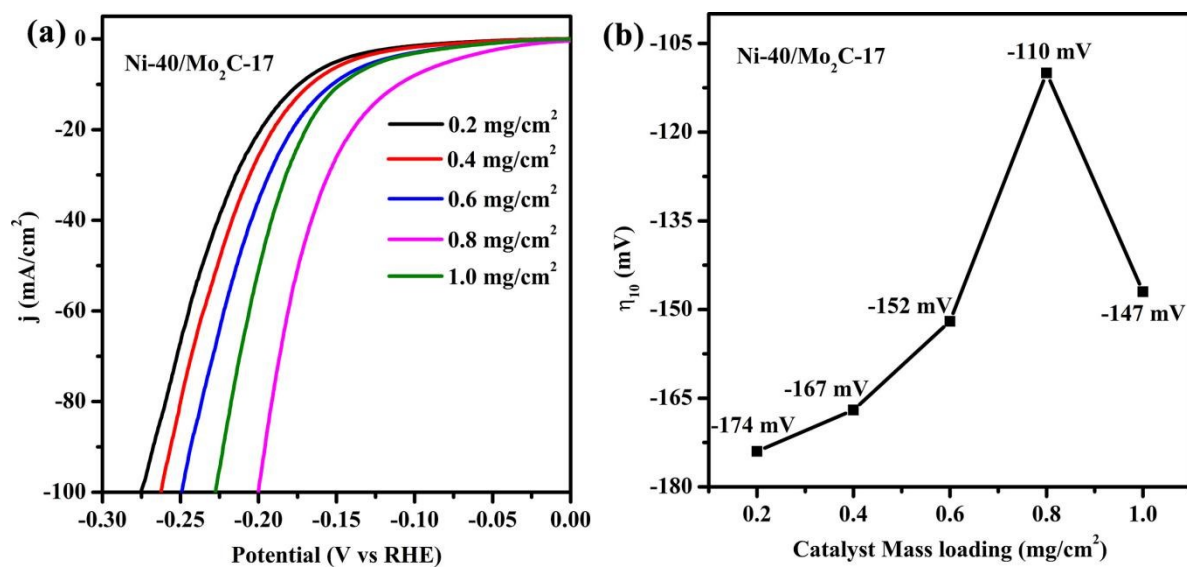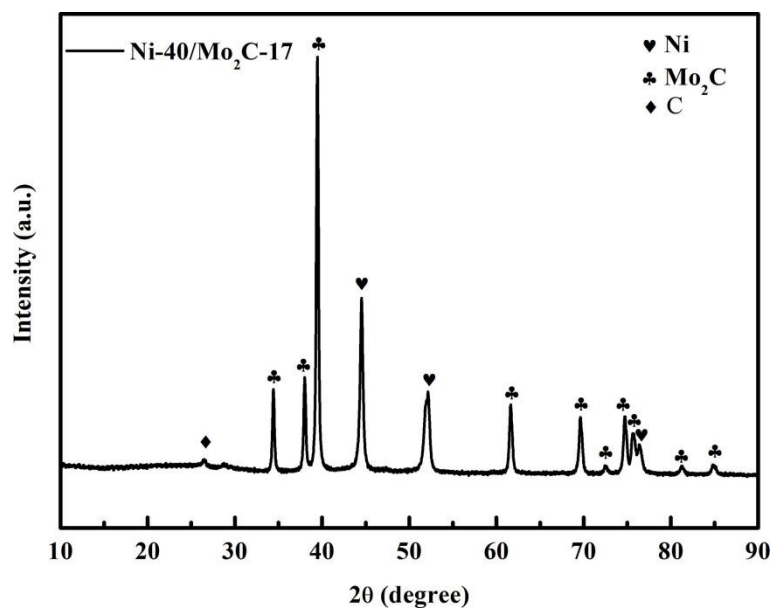

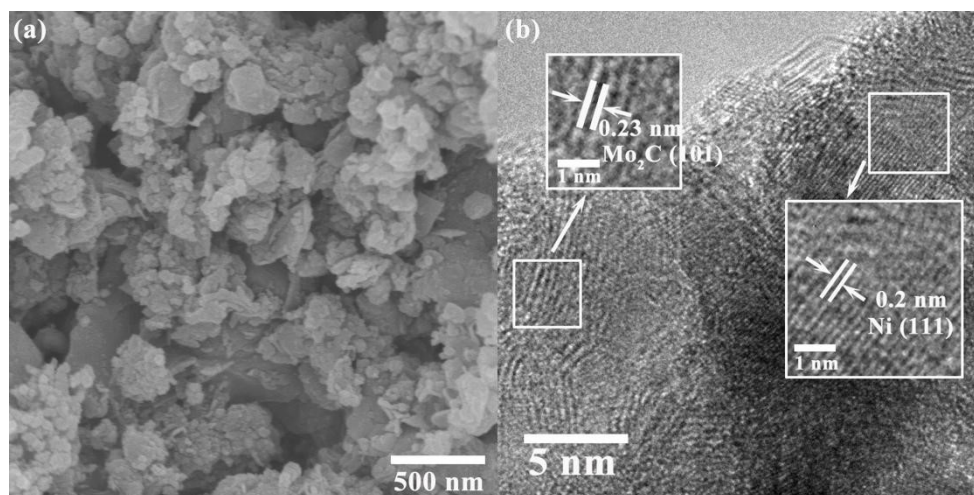**Fig. S8** (a) Polarization curves of Ni-40/Mo_2C-17 under different mass loading, (b) the relationship between mass loading and η_{10} in 1 M KOH.
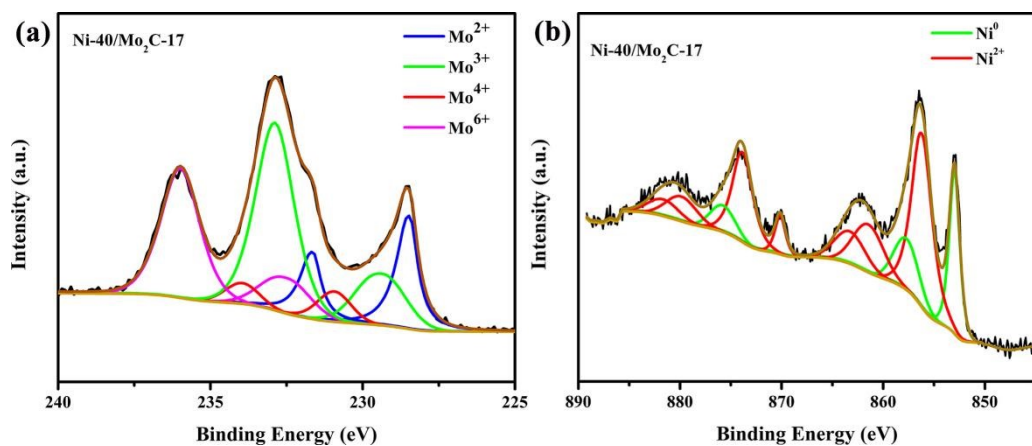
Fig. S9 XRD characterization of Ni-40/Mo$_2$C-17 catalyst after long-term stability test.

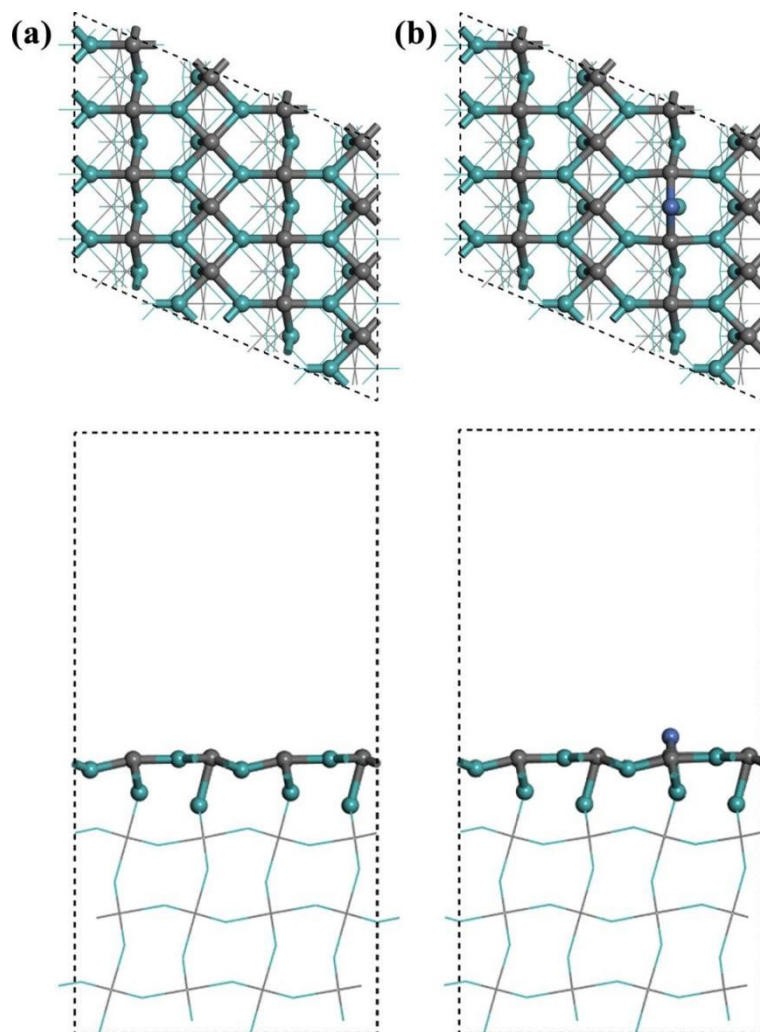**Fig. S10** (a) SEM image of Ni-40/Mo$_2$C-17 after long-term stability test. (b) HRTEM image of Ni-40/Mo$_2$C-17 after long-term stability test.

Fig. S11 (a) Mo *3d* XPS spectra of Ni-40/Mo$_2$C-17 after long-term stability test. (b) Ni *2p* XPS spectra of Ni-40/Mo$_2$C-17 after long-term stability test.

Fig. S12 The optimized structures of (a) clean and (b) Ni doped Mo$_2$C (101) surface.

Table S1 Comparison of the HER performance for Ni-40/Mo$_2$C-17 catalyst with other Mo$_2$C-based or Ni-based catalysts in alkaline electrolytes (1 M KOH).

Catalyst	Loading density (mg cm^{-2})	η_{10} (mV)	Reference
Mo$_2$C-Ni	0.285	372	*New J. Chem.* 2017, 41, 12956
Ni/Mo$_2$C-PC	0.5	179	*Chem. Sci.* 2017, 8, 968
Ni/Mo$_2$C(1:2)-NCNFs	1.4	143	*Adv. Energy Mater.* 2019, 9, 1803185
Mo$_2$C	0.8	190	*Angew. Chem. Int. Ed.* 2012, 51, 1270
Mo$_2$C	0.009	270	*J.Am. Chem. Soc.* 2015, 137, 7035
L-Mo$_2$C	N/A	95.8	*ACS Appl. Mater. Interfaces*, 2018, **10**, 40500
Mo$_2$C-NCNT	3	257	*J. Mater. Chem. A* 2015, 3, 5783
Mo$_2$C/carbon sheets	0.4	178	*ChemSusChem* 2017, 10, 3540
NiO/Ni-CNT	0.28	80	*Nat. Commun.* 2014, 5, 4695
NiFe LDH/NF	N/A	210	*Science* 2014, 345, 1593
NiFe LDH/rGO	0.25	560	*ACS Nano* 2015, 89, 1977
Ni-40/Mo$_2$C-17	0.8	110	This work