Supplementary Information

Anchoring Pt-based alloy on the oxygen-vacancy-defected MXene nanosheet for efficient hydrogen evolution reaction and oxygen reduction reaction

Qin Zhao[a], Yu Zhang[a], Changwang Ke[a], Xiaofei Yang[a], Weiping Xiao[a,b*]

[a] College of Science, Institute of Materials Physics and Chemistry, Nanjing Forestry University, Nanjing 210037, China

[b] Key Laboratory of Advanced Energy Materials Chemistry (Ministry of Education), College of Chemistry, Nankai University, Tianjin 300071, China

*Corresponding author

E-mail address: wpxiao@njfu.edu.cn

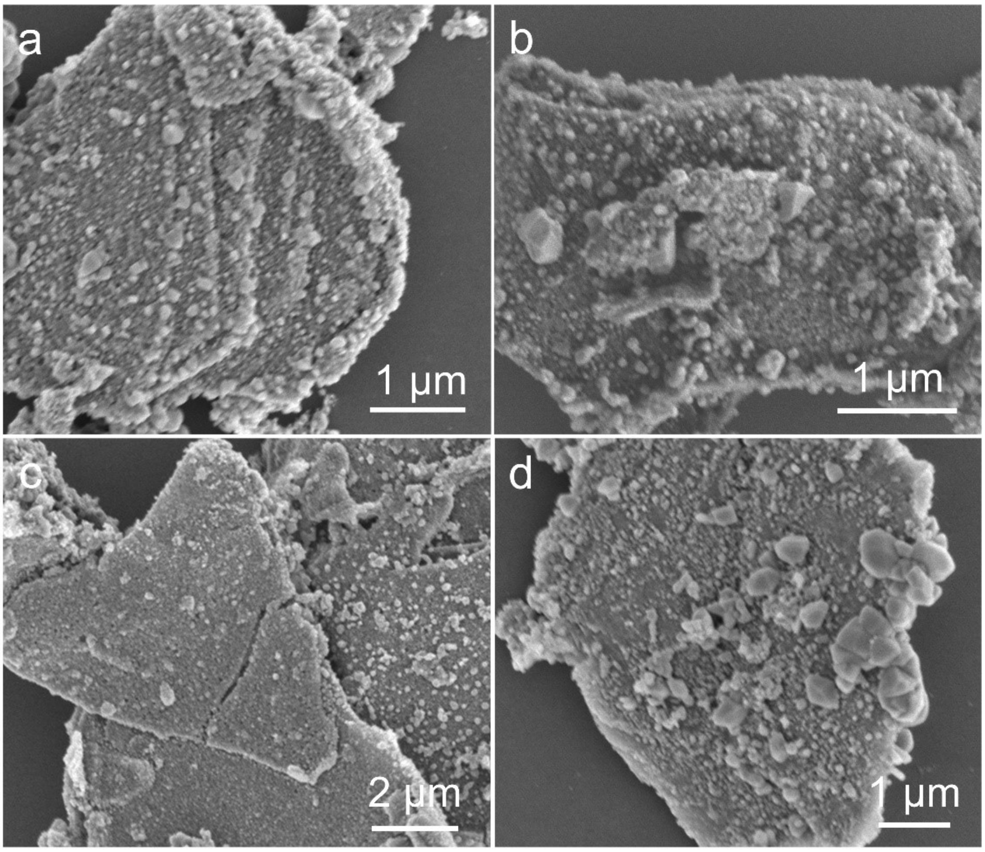

Fig. S1 SEM images of (a) Pt_3Ni/MXene-500, (b) Pt_3Ni/MXene-900, (c) Pt_3Co/MXene-500, (d) Pt_3Co/MXene-900.

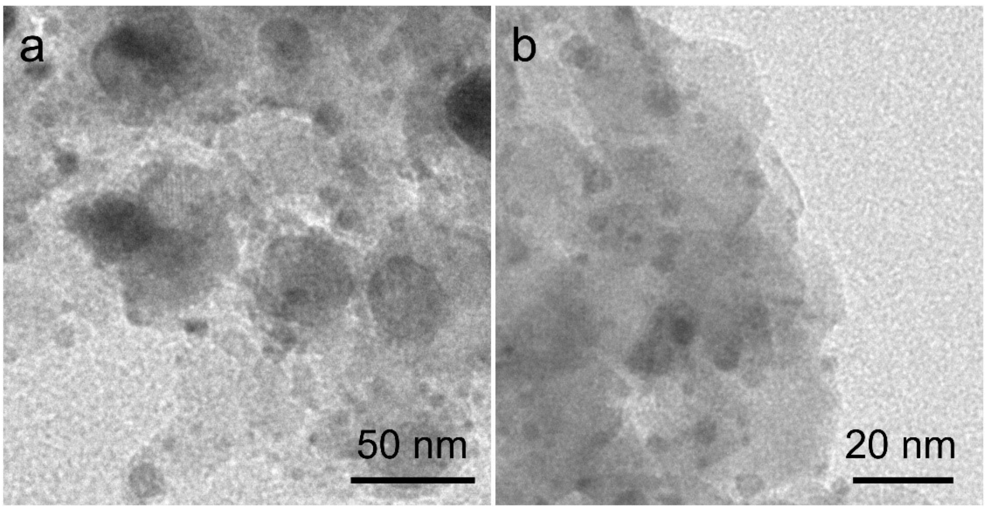

Fig. S2 TEM images of Pt_3Ni/MXene-700.

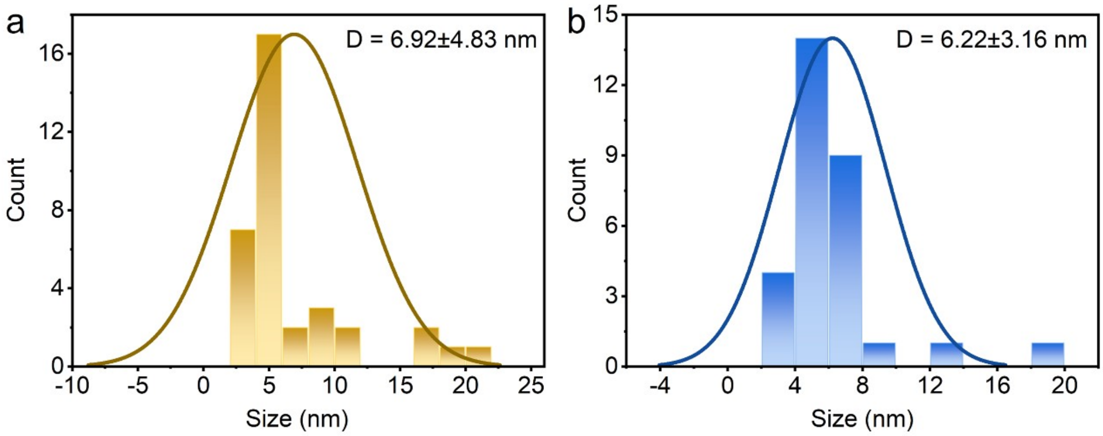

Fig. S3 Particle size distribution of Pt_3Ni/MXene-700 and Pt_3Co/MXene-700 catalyst.

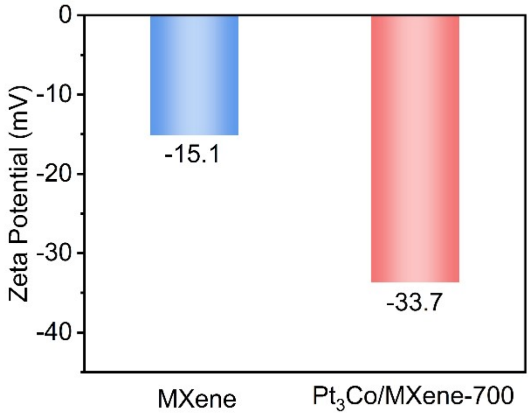

Fig. S4 The zeta potentials of MXene and Pt_3Co/MXene-700.

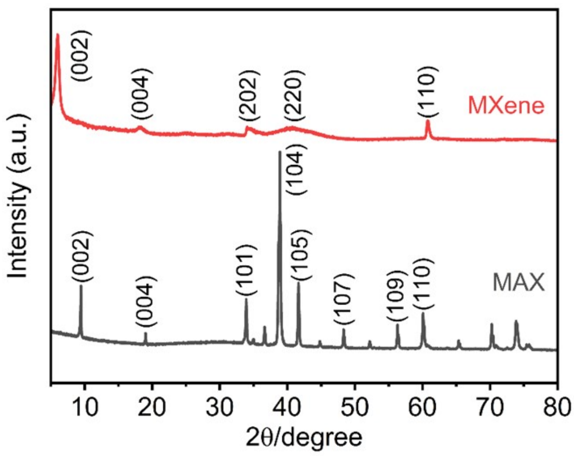

Fig. S5 XRD patterns of MAX and MXene.

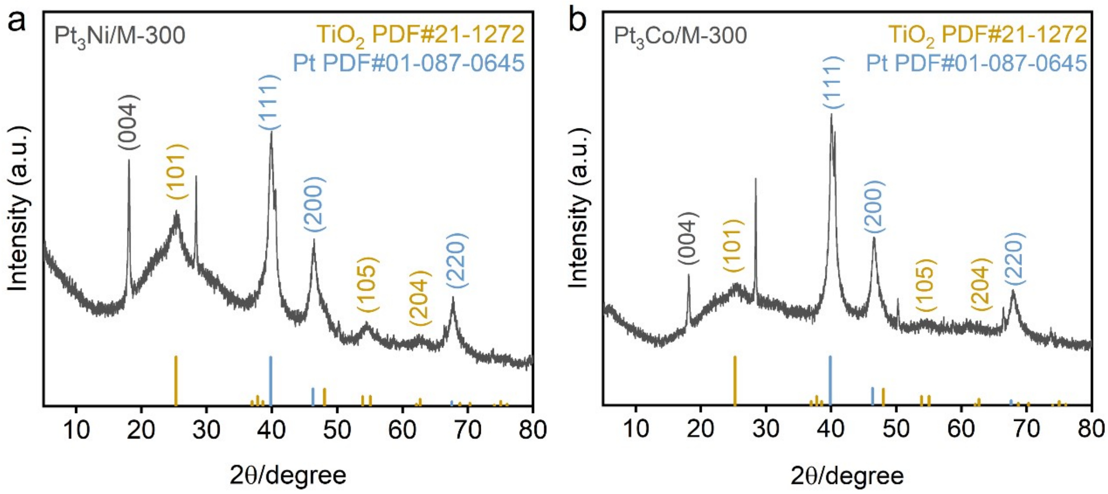

Fig. S6 XRD patterns of (a) Pt_3Ni/MXene-300 and (b) Pt_3Co/MXene-300.

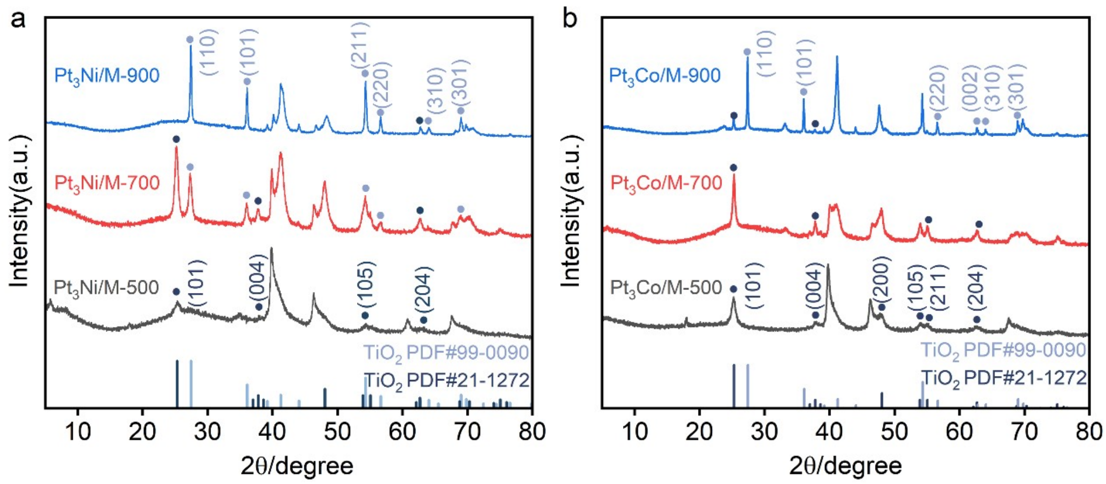

Fig. S7 (a) XRD patterns of Pt_3Ni/MXene-500, 700, 900 catalysts; (b) XRD patterns of Pt_3Co/MXene-500, 700, 900 catalysts.

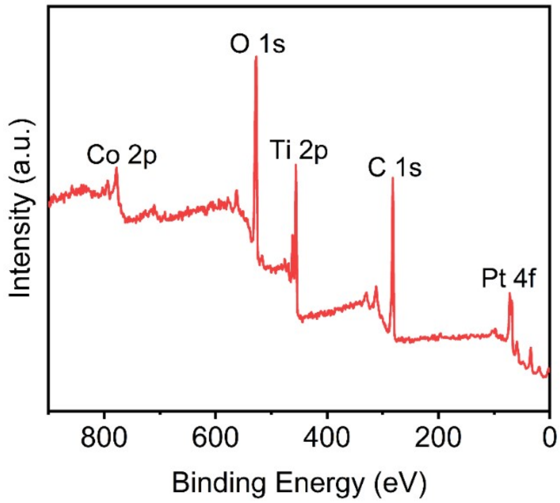

Fig. S8 XPS survey spectra of Pt_3Co/MXene-700 catalyst.

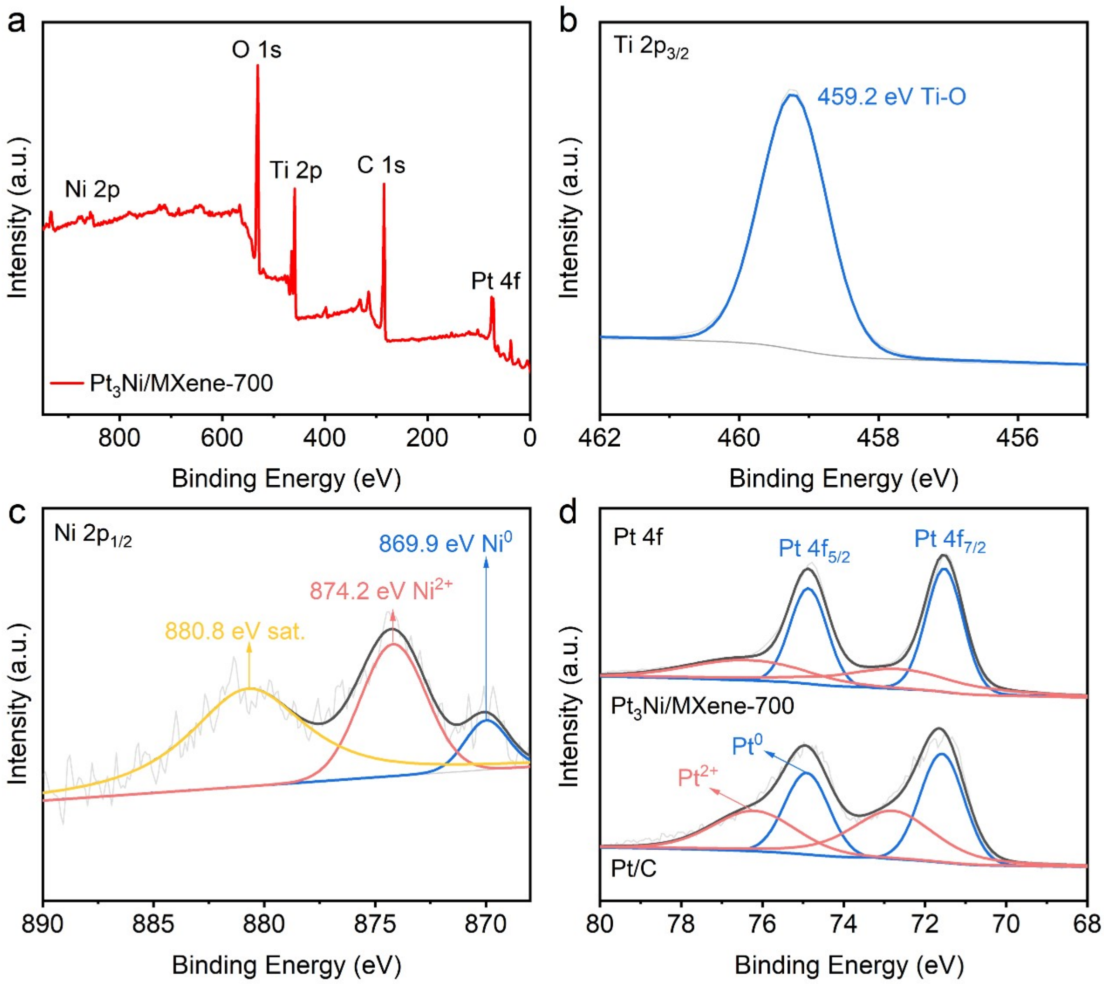

Fig. S9 (a) XPS survey spectra of Pt_3Ni/MXene-700. High-resolution XPS spectra of (b) Ti 2p, (c) Ni 2p and (d) Pt 4f of Pt_3Ni/MXene-700 catalyst.

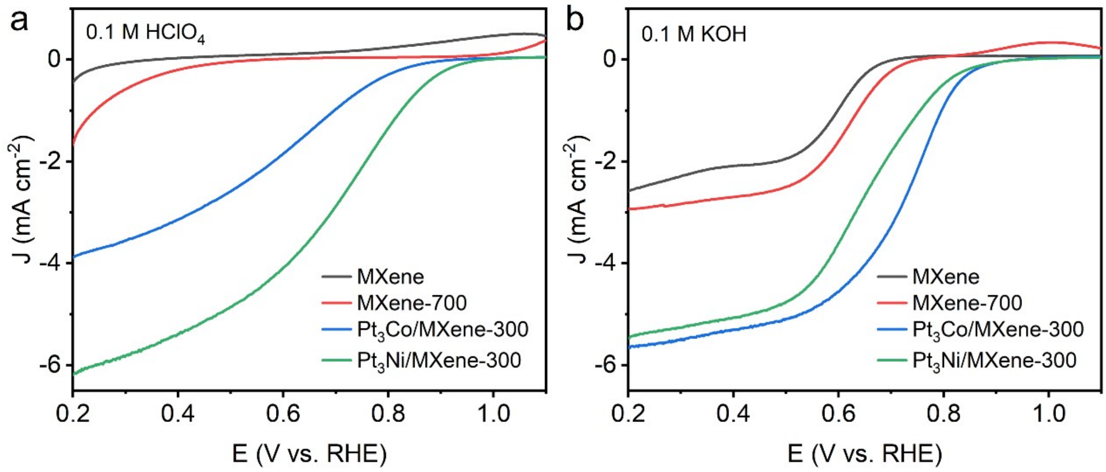

Fig. S10 The ORR performance of MXene, MXene-700, Pt_3M/MXene-300 (M = Co, Ni) in (a) 0.1 M $HClO_4$ and (b) 0.1 M KOH.

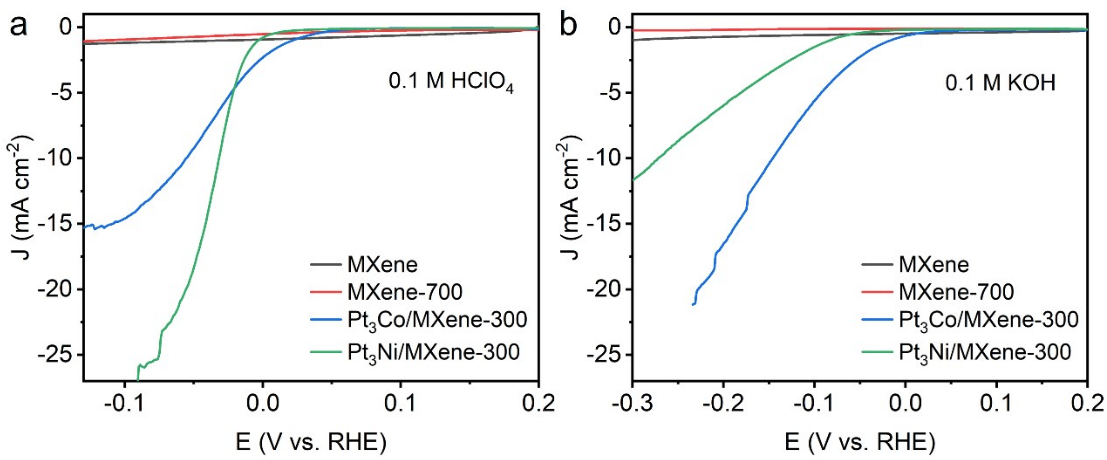

Fig. S11 The HER performance of MXene, MXene-700, Pt_3M/MXene-300 (M = Co, Ni) in (a) 0.1 M $HClO_4$ and (b) 0.1 M KOH.

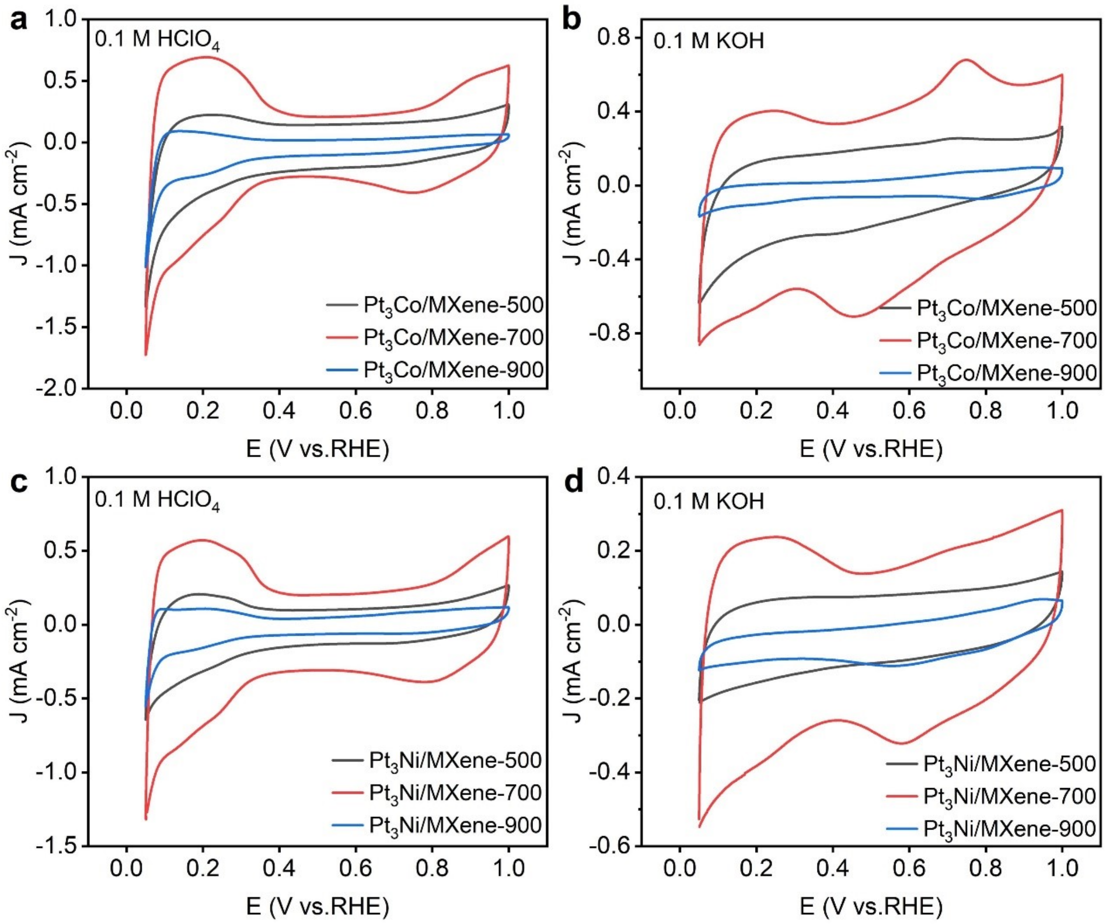

Fig. S12 CV curves in (a) 0.1 M $HClO_4$ and (b) 0.1 M KOH of Pt_3Co/MXene catalysts; CV curves in (c) 0.1 M $HClO_4$ and (d) 0.1 M KOH of Pt_3Ni/MXene catalysts.

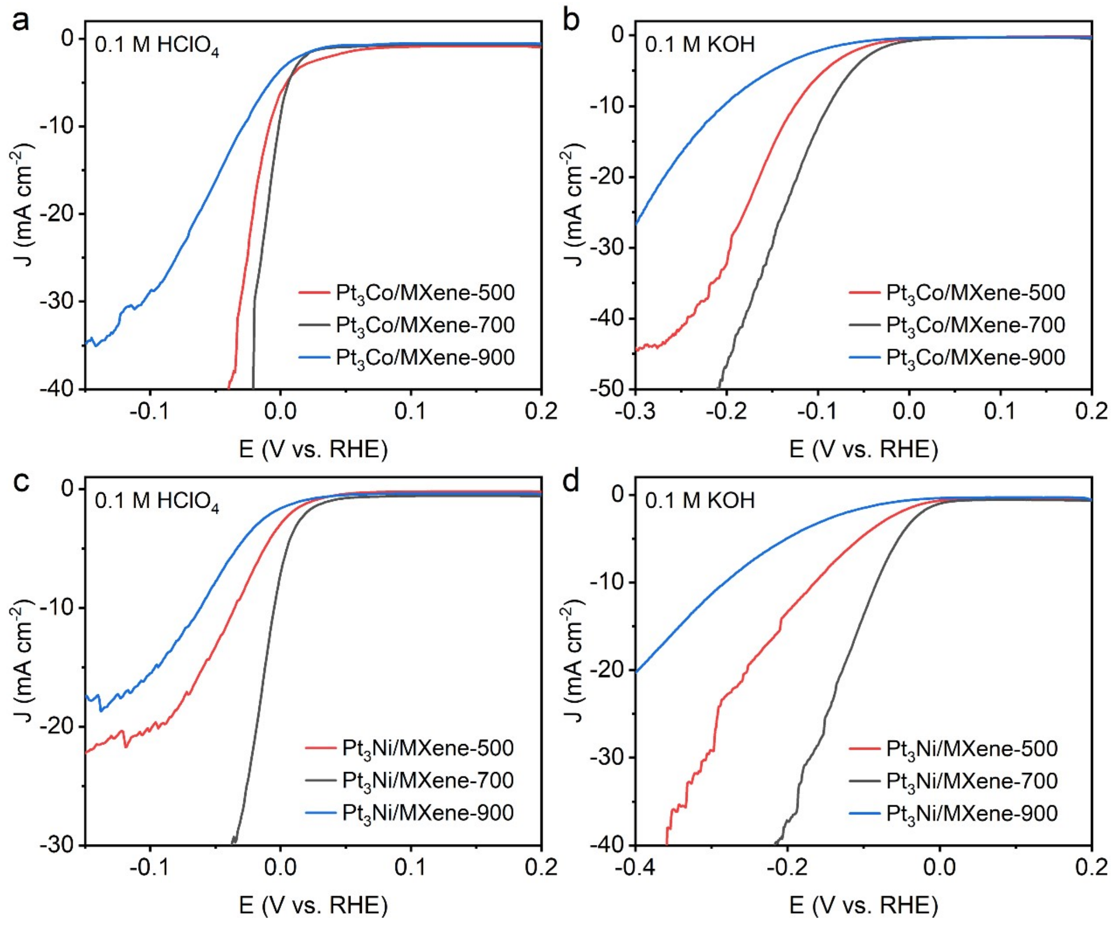

Fig. S13 (a, b) HER performance of Pt_3Co/MXene-500, 700, 900 catalysts in 0.1 M $HClO_4$ and 0.1 M KOH, (c, d) HER performance of Pt_3Ni/MXene-500, 700, 900 catalysts in 0.1 M $HClO_4$ and 0.1 M KOH.

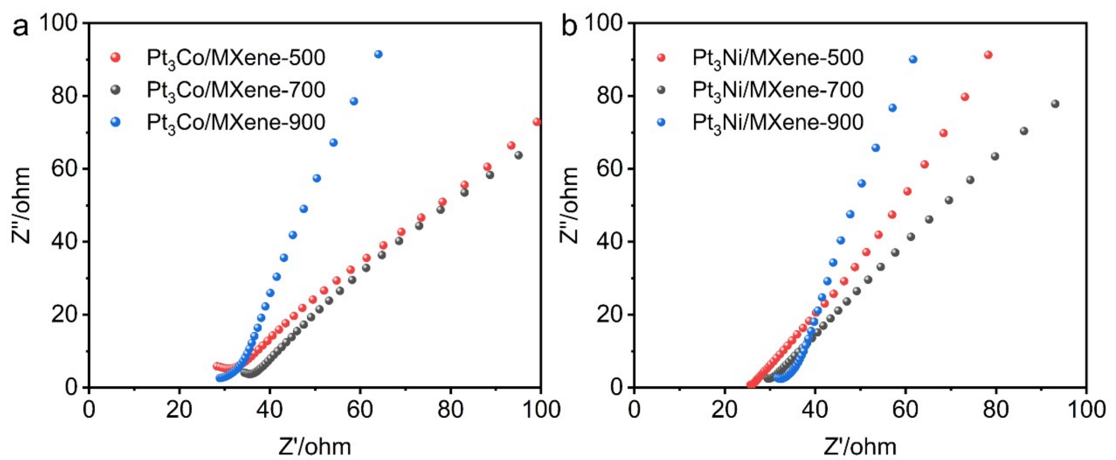

Fig. S14 Nyquist plots of Pt_3M/MXene-500, 700, 900 (M = Co, Ni) in 0.1 M $HClO_4$.

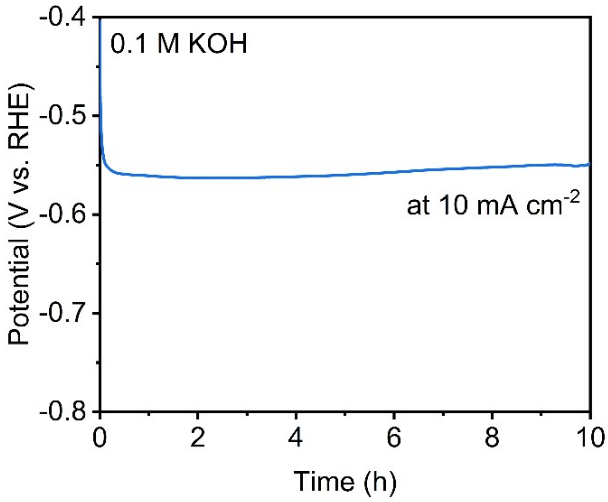

Fig. S15 Chronopotentiometric curve of Pt_3Co/MXene-700 measured at 10 mA cm^{-2} in 0.1 M KOH.

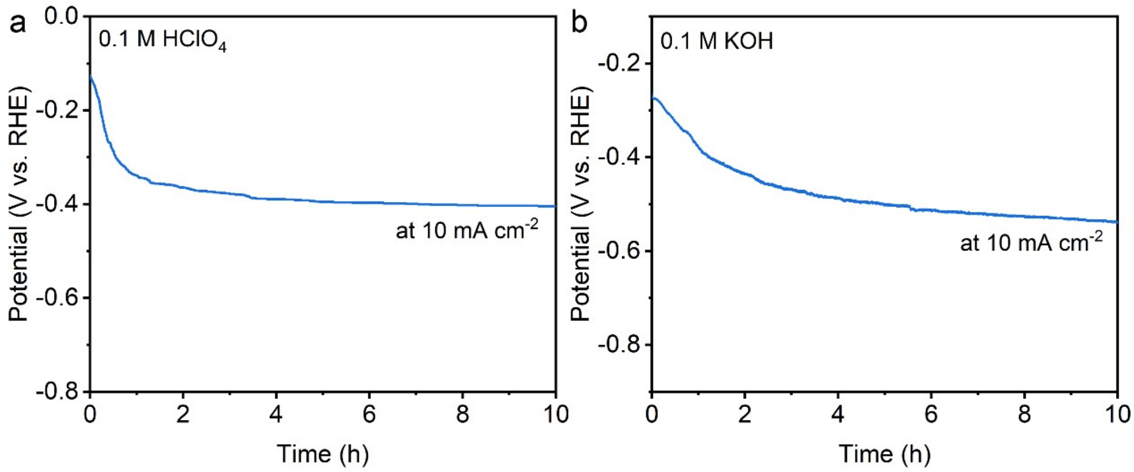

Fig. S16 Chronopotentiometric curve of Pt_3Ni/MXene-700 measured at 10 mA cm^{-2} in 0.1 M $HClO_4$ and KOH.

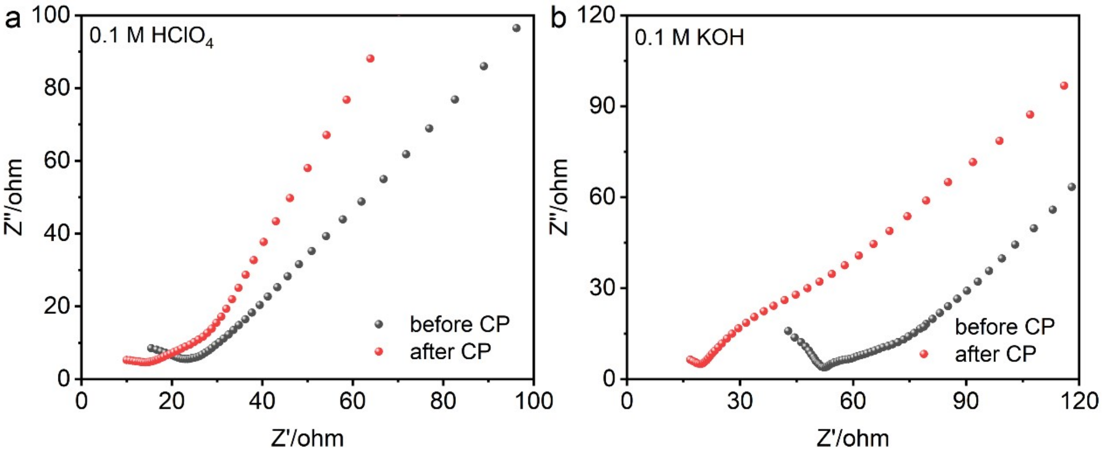

Fig. S17 Nyquist plots of Pt_3Co/MXene-700 before and after stability testing in 0.1 M $HClO_4$ and 0.1 M KOH.

Table S1. The degree of Pt shrinkage in Pt alloys of Pt_3Co/MXene-700 and Pt_3Ni/MXene-700 catalysts.

Catalysts	**a=b=c**	**Degree of lattice contraction**
Pt	3.92	\
Pt_3Co/MXene-700	3.878	10.71%
Pt_3Ni/MXene-700	3.911	2.3%

Table S2. Comparison of the ORR performance of recent reported catalysts in 0.1 M $HClO_4$ (H) and 0.1 M KOH (OH) solution.

Catalysts	**$E_{1/2}$ (H) (*vs.* RHE)**	**Tafel slope**	**$E_{1/2}$ (OH) (*vs.* RHE)**	**Tafel slope**	**Ref.**
Pt_3Co/MXene-700	0.897 V	88.77	0.901 V	69.89	This work
Pt_3Ni/MXene-700	0.889 V	104.22	0.897 V	91	This work
Pt/MXene	0.892 V	95.82	\	\	1
Fe-N-C@MXene	0.777 V	78	0.887 V	88	2
TiCN-BCN-Co	\	\	0.81 V	90.8	3
NiCo-LDH/Ti_3C_2	\	\	0.66 V	90	4
$MnCo_2O_4$/NGQD/MXene	\	\	0.876 V	63	5
Fe/Co-CNT@MXene	\	\	0.85 V	76	6
PtNi/NC	\	\	0.82 V	80.5	7
Co/Co_3O_4@C	0.823 V	85.8	0.672 V	100.4	8
Pt_{SA}-PtCo NCs/N-CNT-900	0.89 V	\	0.86 V	74	9
Pt_4Co@NC-900	0.88 V	68	\	\	10
PtCoNG-3500-600/900	0.86 V	\	\	\	11
PtCu HNF	0.87 V	78.8	\	\	12
Co/CeO_2	\	\	0.75 V	80	13

Table S3. Comparison of the HER performance of recent reported catalysts in 0.1 M $HClO_4$ (H) and 0.1 M KOH (OH) solution.

Catalysts	**Overpotential (η_{10}, H)**	**Tafel slope**	**Overpotential (η_{10}, OH)**	**Tafel slope**	**Ref.**
Pt_3Co/MXene-700	1.2	27.11	82.5	76.01	This work
Pt_3Ni/MXene-700	4.6	36.78	88.3	76.12	This work
Pt/$Ti_3C_2T_x$-550	32.7	32.3	\	\	14
$IrCo_{0.14}$	16	28.8	\	\	15
$IrCo_{0.65}$	17	35.3	\	\	16
Pd/OMC	167	68	\	\	17
Pt@PDG4	\	\	55	79.2	18
MoS_2-CoNi$(OH)_2$	\	\	178	60.9	19
Co/NGC-3	\	\	293	130	20
CMCO NWs	140	39	\	\	21
NiS_2/PtNi NWs	15	20	\	\	22
Pd/OMC	167	62	\	\	23

References

1 Z. Zhang, C. Liu, Y. Dai, B. Liu, P. Guo, F. Tu, M. Ma, L. Shen, Z. Zhao, Y. Liu, Y. Zhang, L. Zhao and Z. Wang, *ACS Appl. Energy Mater.*, 2022, **5**, 14957–14965.

2 W.T. Wang, N. Batool, T. H. Zhang, J. Liu, X. F. Han, J. H. Tian and R. Yang, *J. Mater. Chem. A*, 2021, **9**, 3952–3960.

3 Y. Wang, F. Gu, L. Cao, L. Fan, T. Hou, Q. Zhu, Y. Wu and S. Xiong, *Int J Hydrogen Energy*, 2022, **47**, 20894–20904.

4 G. L. Li, S. Cao, Z. F. Lu, X. Wang, Y. Yan and C. Hao, *Appl. Surf. Sci.*, 2022, **591**, 153142.

5 M. Faraji, S. Yousefzadeh, M. F. Nassar and M. M. A. Zahra, *J. Alloy Compd.*, 2022, **927**, 167115.

6 C. Zhang, H. Dong, B. Chen, T. Jin, J. Nie and G. Ma, *Carbon*, 2021, **185**, 17–26.

7 X. Chen, J. Guo, J. Liu, Z. Luo, X. Zhang, D. Qian, D. Sun-Waterhouse and G. I. N. Waterhouse, *J. Phys. Chem. Lett.*, 2023, **14**, 1740–1747.

8 Q. Zhang, X. Zhao, X. Miao, W. Yang, C. Wang and Q. Pan, *Int. J. Hydrogen Energy*, 2020, **45**, 33028–33036.

9 W. Chen, X. Zhu, W. Wei, H. Chen, T. Dong, R. Wang, M. Liu, K. (Ken) Ostrikov, P. Peng and S. Zang, *Small*, 2023, 2304294.

10 N. Zhou and Y. Li, *Int. J. Hydrogen Energy*, 2021, **46**, 37884–37894.

11 L. Sun, Y. Qin and Y. Yin, *J. Power Sources*, 2023, **562**, 232758.

12 G. Ma, X. Zhao, J. Wang, G. Qin, Z. Lu, X. Yu, L. Li, X. Zhang and X. Yang, *J. Electroanal. Chem.*, 2022, **922**, 116756.

13 Z. Liu, J. Wan, M. Li, Z. Shi, J. Liu and Y. Tang, *Nanoscale*, 2022, **14**, 1997–2003.

14 Z. Li, Z. Qi, S. Wang, T. Ma, L. Zhou, Z. Wu, X. Luan, F. Y. Lin, M. Chen, J. T. Miller, H. Xin, W. Huang and Y. Wu, *Nano Lett.*, 2019, **19**, 5102–5108.

15 W. Gao, Q. Xu, Z. Wang, M. Wang, X. Ren, G. Yuan and Q. Wang, *Electrochim. Acta*, 2020, **337**, 135738.

16 L. Fu, X. Zeng, G. Cheng and W. Luo, *ACS Appl. Mater. Interfaces*, 2018, **10**, 24993–24998.

17 J. G. Kim, B. Lee, N. N. T. Pham, S. G. Lee and C. Pak, *J. Ind. Eng. Chem.*, 2020, **89**, 361–367.

18 Z. Li, F. Han, Z. Liu, Q. Peng, Q. D. Wang, M. Sun and G. J. Kang, *New J. Chem.*, 2021, **45**, 21670–21675.

19 Y. Zhang, L. Xue, C. Liang, Y. Chen, J. Liu, C. Shen, Q. Li, Y. Duan, L. Yao, H. Zhang, Y. Cai, C. Tan and Z. Luo, *Appl. Surf. Sci.*, 2021, **561**, 150079.

20 J. Li, Y. Kang, D. Liu, Z. Lei and P. Liu, *ACS Appl. Mater. Interfaces*, 2020, **12**, 5717–5729.

21 Q. Li, K. Liu, S. Gui, J. Wu, X. Li, Z. Li, H. Jin, H. Yang, Z. Hu, W. Liang and L. Huang, *Nano Res.*, 2022, **15**, 2870–2876.

22 G. Wang, X. Huang, H. G. Liao and S. G. Sun, *Energ. Fuel.*, 2021, **8**, 6928–6934.

23 J. G. Kim, B. Lee, N. N. T. Pham, S. G. Lee and C. Pak, *J. Ind. Eng. Chem.*, 2020, **89**, 361–367.