Electronic Supplementary Material (ESI) for New Journal of Chemistry.
This journal is © The Royal Society of Chemistry and the Centre National de la Recherche Scientifique 2020

NEW J CHEM

Electronic Supplementary Information

Experimental and theoretical investigation on MoS_2/MXene heterostructure as an efficient electrocatalyst for PH-universal hydrogen evolution reaction

Le Hu[a], Yuyun Sun[a], Shi-Jing Gong[a], Hui Zong[a], Ke Yu*[a,b] and Ziqiang Zhu[a]

[a] *Key Laboratory of Polar Materials and Devices (MOE), Department of Electronics, East China Normal University, Shanghai 200241, China*

[b] *Collaborative Innovation Center of Extreme Optics, Shanxi University, Taiyuan, Shanxi 030006, China*

* Corresponding Author:

Tel: +86-21-54345198.

E-mail address: yk5188@263.net.

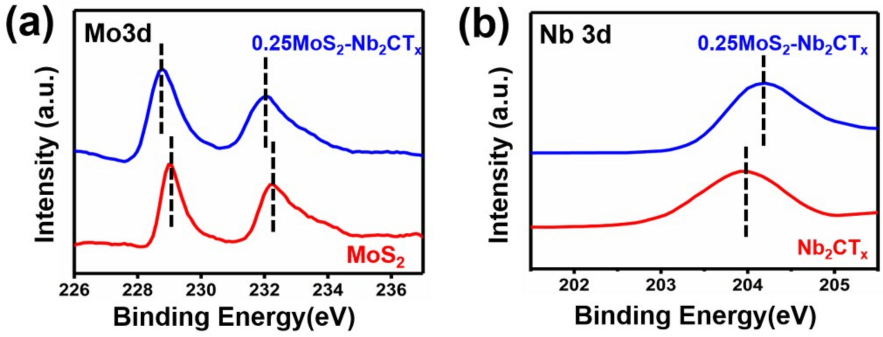

Fig. S1 (a) Mo 3d XPS spectra of 0.25 MoS_2-Nb_2CT_x heterostructure and MoS_2. (b) Nb 3d XPS spectra of 0.25 MoS_2-Nb_2CT_x heterostructure and Nb_2CT_x.

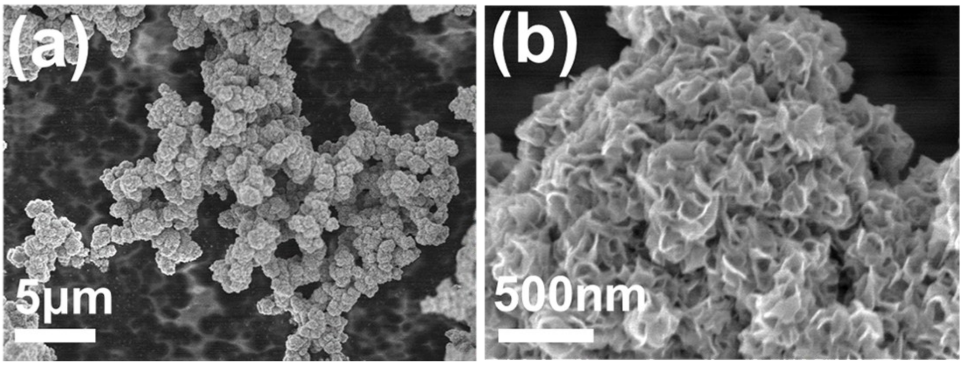

Fig. S2 SEM images of MoS_2.

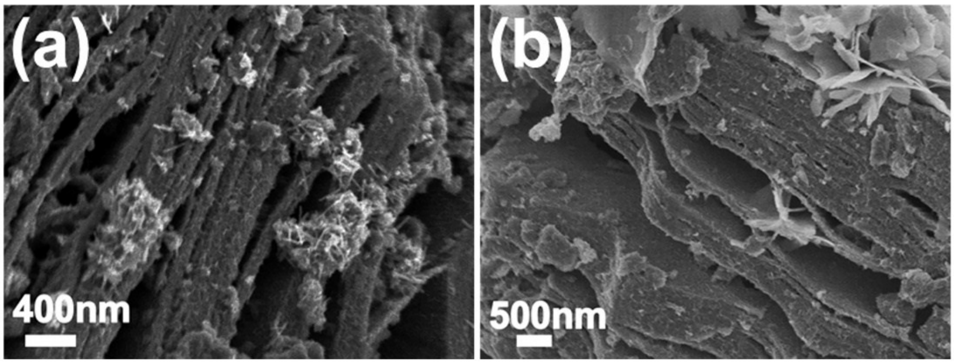

Fig. S3 SEM images of 0.15 MoS_2-Nb_2CT_x and 0.35 MoS_2-Nb_2CT_x heterostructures: (a) SEM image of 0.15 MoS_2-Nb_2CT_x heterostructure. (b) SEM image of 0.35 MoS_2-Nb_2CT_x heterostructure.

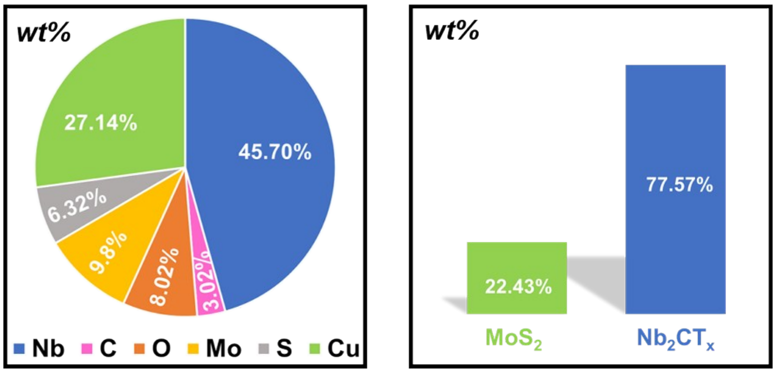

Fig. S4 Mass ratio diagram of elements and chemical composition in 0.25 MoS_2-Nb_2CT_x sample. Because the proportion of Al element is only 0.12%, it is not exhibited in the figure.

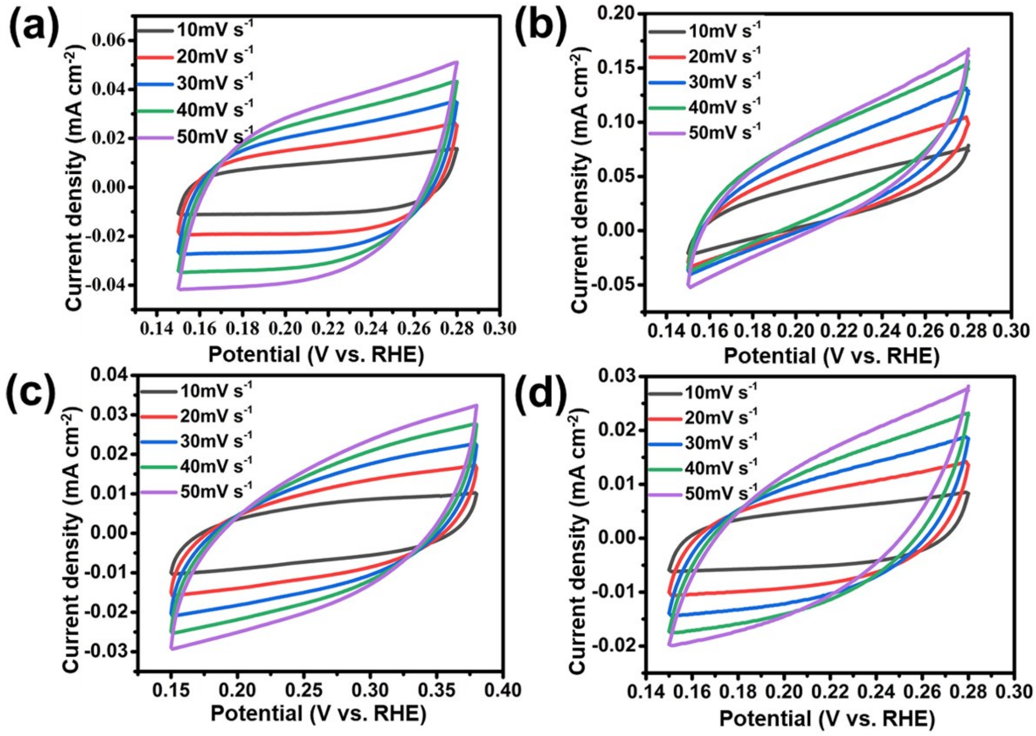

Fig. S5 CV Cyclic voltammetry curves of MoS_2, Nb_2CT_x, 0.15 MoS_2-Nb_2CT_x, and 0.35 MoS_2-Nb_2CT_x: (a) CV Cyclic voltammetry curve of MoS_2, (b) CV Cyclic voltammetry curve of Nb_2CT_x, (c) CV Cyclic voltammetry curve of 0.15 MoS_2-Nb_2CT_x, (d) CV Cyclic voltammetry curve of 0.35 MoS_2-Nb_2CT_x.

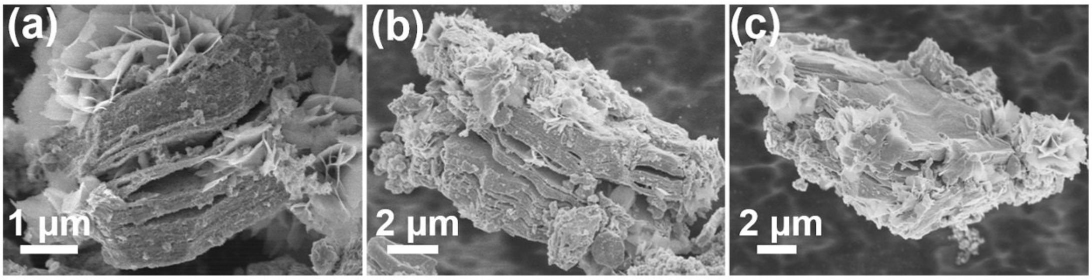

Fig. S6 SEM images of 0.25 MoS_2-Nb_2CT_x before and after the cycles.

(a) SEM image of 0.25 MoS_2-Nb_2CT_x before the cycles. (b) SEM image of the composite after the potential sweeps for 3000 cycles in acidic medium. (c) SEM image of the composite after the potential sweeps for 3000 cycles in alkaline medium.

Table S1. Comparison of HER performances for MoS_2-Nb_2CT_x with related MoS_2-based catalysts.

Catalyst	Overpotential (mV)	Tafel slope (mV dec^{-1})	R_{ct}	Electrolyte	Reference
MoS_2-Nb_2CT_x	127	56.2	63.1	0.5 M H_2SO_4	This work
MoS_2-$Ti_3C_2T_x$	152	70	-	0.5 M H_2SO_4	1
MoS_2-GF	157	93	47.3	0.5 M H_2SO_4	2
Ni@NC/MoS_2-P	325	118.2	28.6	0.5 M H_2SO_4	3
Cu-MoS_2/rGo	244	127	-	0.5 M H_2SO_4	4
CoP/CN @ MoS_2	144	69	-	0.5 M H_2SO_4	5
MoS_2-Nb_2CT_x	141	93.4	231.4	1 M KOH	This work
$(NiFe)_x$-MoS_2	285	94	-	1 M KOH	6
MoS_2-$Co(OH)_2$	179	62	-	1 M KOH	7
MoS_2 @ 3DC	252	102.8	316.3	1 M KOH	8
Fe-MoS_2	163	181	-	1 M KOH	9
Co-MoS_2	215	153	175	1 M KOH	10
Ni-P/MoS_2	155	108	2758	1 M KOH	11

REFERENCES

1 J. Liu, Y. Liu, D. Xu, Y. Zhu, W. Peng, Y. Li, F. Zhang and X. Fan, *Appl. Catal. B*, 2019, **241**, 89-94.
2 B. Liu, S. Wang, Q. Mo, L. Peng, S. Cao, J. Wang, C. Wu, C. Li, J. Guo, B. Liu, W. Chen and Y. Lin, *Electrochim. Acta*, 2018, **292**, 407-418.
3 S. A. Shah, X. Shen, M. Xie, G. Zhu, Z. Ji, H. Zhou, K. Xu, X. Yue, A. Yuan, J. Zhu and Y. Chen, *Small*, 2019, **15**, 1804545.
4 F. Li, L. Zhang, J. Li, X. Lin, X. Li, Y. Fang, J. Huang, W. Li, M. Tian, J. Jin and R. Li, *J. Power Sources*, 2015, **292**, 15-22.
5 J. G. Li, K. Xie, H. Sun, Z. Li, X. Ao, Z. Chen, K. K. Ostrikov, C. W. Wang and W. Zhang, *Appl. Mater. interfaces*, 2019, **11**, 36649-36657.
6 C. Liu, Y. Guo, Z. Yu, H. Wang, H. Yao, J. Li, K. Shi and S. Ma, *Nanotechnology*, 2020, **31**, 035403.
7 Y. Luo, X. Li, X. Cai, X. Zou, F. Kang, H. M. Cheng and B. Liu, *ACS Nano*, 2018, **12**, 4565-4573.
8 L. Diao, B. Zhang, Q. Sun, N. Wang, N. Zhao, C. Shi, E. Liu and C. He, *Nanoscale*, 2019, **11**, 21479-21486.
9 J. Zhang, T. Wang, P. Liu, S. Liu, R. Dong, X. Zhuang, M. Chen and X. Feng, *Energy Environ. Sci.*, 2016, **9**, 2789-2793.
10 J. Liang, C. Ding, J. Liu, T. Chen, W. Peng, Y. Li, F. Zhang and X. Fan, *Nanoscale*, 2019, **11**, 10992-11000.
11 J. He, L. Song, J. Yan, N. Kang, Y. Zhang and W. Wang, *Metals*, 2017, **7**, 211.